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COMMUNICATION OF NUCLEAR DATA PROGRESS

No. 9 (1993)

Chinese Nuclear Data Center

China Nuclear Information Centre

Atomic Energy Press

Beijing, June 1993

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EDITORIAL NOTE

This is the ninth issue of *Communication of Nuclear Data Progress* (CNDP), in which the nuclear data progress in China during the last year is carried. In addition, it includes optical model parameters for both small angles and larger angles elastic scattering, n–T phase shift analyses, forbidden angular region of secondary particle emission, introduction to codes CMUP2 and CFUP1, diffusion process of nuclear fission, techniques used for charged particle evaluation at CNDC, evaluation of neutron nuclear data for ^{7}Li and revision on recommended data of ^{238}U for CENDL–2, Chinese Evaluated Nuclear Parameter Library (CENPL) (II) and computer program library at CNDC, covariance data evaluation for experimental data and several examples of least squares combination for derived data, and calculation of thermal neutron scattering law for anisotopic microcrystal etc.

For a limited experience and knowledge, there might be some shortcomings and errors, welcome to make comments about them.

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CONTENTS

I EXPERIMENTAL MEASUREMENT

OPTICAL MODEL PARAMETERS AND FAST NEUTRON SMALL ANGLES SCATTERING CROSS SECTIONS

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ABSTRACT

The differential cross sections of 14.8 MeV (or 14.7 MeV) neutrons scattered from ^{238}U, Pb, Ni, Fe, Cr and Al between 2.5° to 16° measured by Tsinghua University and those cross sections in the larger angle region measured by others are analysed with spherical optical model or coupled channels model (code ECIS79). A set of global optical model parameters were obtained at 14.8 MeV neutron energy for mass number between 27 and 233. The measured and calculated results are compared and discussed.

INTRODUCTION

It is well known that in ~ 14 MeV neutron–nucleus elastic scattering process, most of the scattered neutrons are in small angle region, so the precise knowledge of the differential cross sections at small angles is important. But the data for the angles smaller than 15° are very scarce because of the difficulties in geometrical arrangement of most measurements. By use of the optical model, the differential cross sections at small angles can be calculated. But most of the optical model parameters (OMP) published in the past were obtained without experimental data in the small angle regions. They can not be assured fitting the

small angle scattering data very well. For example, the comparisons[1, 2] of the experimental data with the calculated data using different OMPs for Cr and ^{238}U are given in Figs. 1 and 2, respectively; there is quite large discrepancy in the small angle regions between the predictions with different OMPs. What are the best global OMPs which can perfectly predict experimental data of elastic scattering differential cross sections both in the small angle and in the larger angle regions ? Hence it is necessary to measure systematically the small angle scattering cross sections, and to analyze them using optical model. Finally, a set of OMP should be obtained, which can describe the angular distributions quite well both in the small angle region and larger angle region.

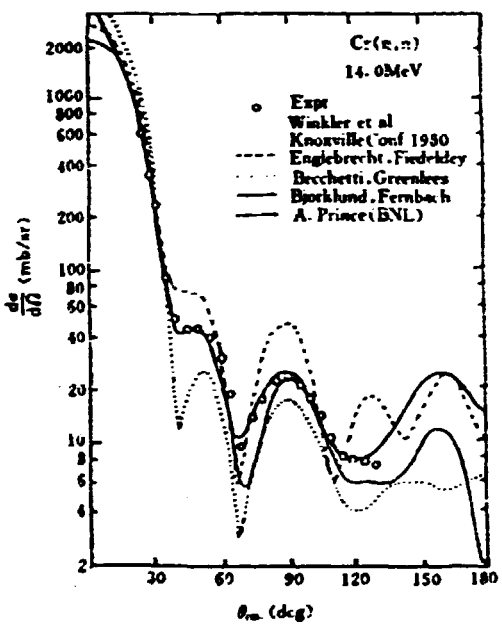

Fig. 1 Comparison of experimental data with calculated data using various OMP for Cr

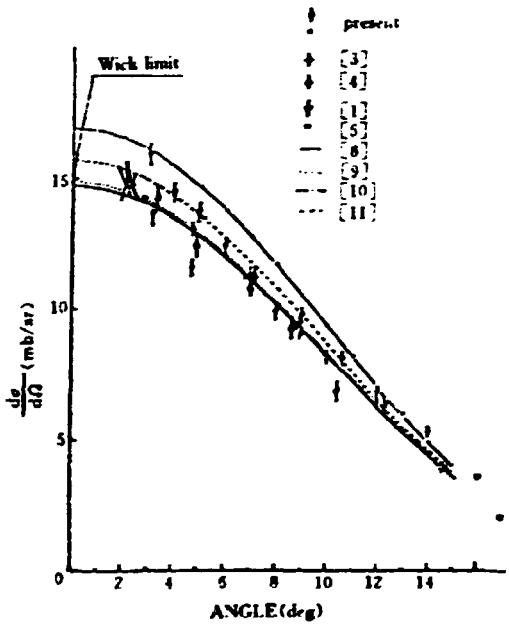

Fig. 2 Comparison of experimental data with calculated data using various OMP for U

1 MEASURED RESULTS

The neutron scattering differential cross sections between 2.5° and 16° were measured at Tsinghua University in the past several years. Which have been published in Refs. [2~6].

The measurements were carried out on Cockcroft Walton accelerator, with neutron produced by $^{3}H(d,n)^{4}He$ reaction at E_n = 14.7 MeV for U and

Pb, E_n = 14.8 MeV for Ni, Fe, Cr and Al.

A part of the results are shown in table 1 to table 4. All of the data in the tables are in lab. systems.

Table 1 differential cross sections for ^{238}U

θ (deg.)	2.2	3.3	4.9	7.0	8.9	10.4	12.3	14.6
σ (b/sr)	14.9±0.8	14.6±0.6	12.3±0.6	11.4±0.5	9.3±0.4	6.8±0.4	6.2±0.3	3.9±0.3

Table 2 Differential cross sections for Pb

θ (deg.)	3.0	4.5	6.0	7.5	9.0
σ (b/sr)	13.2±0.7	12.1±0.7	11.2±0.6	10.8±0.6	9.0±0.5

Table 3 Differential cross sections for Fe, Ni and Cr (b/sr)

θ	2.5	4.0	6.0	8.0	10.0	12.0	14.0	16.0
Fe	3.31±0.13	3.19±0.10	2.68±0.08	2.36±0.07	2.38±0.07	2.11±0.06	1.62±0.11	1.30±0.10
Ni	3.43±0.14	3.29±0.13	3.02±0.11	2.81±0.10	2.76±0.10	2.18±0.08	2.25±0.16	1.32±0.11
Cr	2.88±0.14	2.77±0.11	2.66±0.09	2.38±0.08	2.36±0.08	2.10±0.07	1.89±0.13	1.44±0.12

Table 4 Differential cross sections for Al

θ (deg.)	2.6	3.4	4.9	6.6	8.6
σ (b/sr)	1.38±0.10	1.36±0.10	1.36±0.10	1.31±0.10	1.20±0.10

2 DATA ANALYSES

The differential elastic scattering cross sections were analyzed for each nucleus with spherical optical model or coupled channel code ECIS79. The differential cross sections those have been analyzed are included in both small angle regions and larger angle regions.

The data of differential cross sections in the larger angle region for U, Pb, Fe, Ni, Cr and Al were compiled and evaluated. The best ones (Refs. [7~14]) have been chosen.

Based on the analysis of individual nucleus, the global optical model parameters were searched. First, substitute the geometry parameters of each nucleus with the average geometry parameters and keep them fixed, the potential parameters were adjusted for each nucleus to search for the optimum ones.

If the satisfactory OMP could not found, then the geometry parameters would be changed and the above procedures were repeated until a set of parameters were obtained which could fit each angular distribution satisfactorily. It would be necessary to introduce the asymmetry term $(N-Z)/A$ dependence. The relations between real potential, imaginary surface term and $(N-Z)/A$ for each nucleus were investigated, and then the OMP were readjusted again and again. Finally a set of global OMP was obtained as follows :

$$r_c = 1.20 \quad r_v = 1.20 \quad r_s = 1.26 \quad r_{so} = 1.20$$
$$a_o = 0.70 \quad a_v = 0.62 \quad a_s = 0.62 \quad a_{so} = 0.70$$
$$V_o = 50.42 - 26.0 \times (N-Z)/A$$
$$W_v = 1.42 \quad W_s = 6.077 - 5.0 \times (N-Z)/A \quad V_{so} = 6.04$$

The term $(N-Z)/A$ of each natural sample is calculated as follows :

Pb — the weight average of ^{208}Pb, ^{207}Pb and ^{206}Pb
Ni — the weight average of ^{58}Ni and ^{60}Ni
U — ^{238}U, Fe — ^{56}Fe, Cr — ^{52}Cr, Al — ^{27}Al

The quadruple deformation parameters β_2 for ^{238}U, Ni, Fe, Cr and Al are 0.217, 0.19, 0.24, 0.16 and −0.36, respectively. The hexadecapole deformations β_4 for ^{238}U is 0.082.

In order to test whether the above parameters are suitable for nuclei with mass number between 60 and 100. A comparison between the calculated data using the above parameters and the experimental data (Refs. [12, 13]) of ^{93}Nb have been carried out. As a further test of the data in the small angle region those have been measured and analyzed in Tsinghua University, Wick limit provides a reference value of the differential elastic scattering cross section at zero degree (σ_{el} (0°)). That is

$$\sigma_{el}(0^\circ) \geq (\frac{k\sigma_T}{4\pi})^2$$

where σ_T is the total cross section. Its values were taken from JENDL-3. The comparison of calculated data in this work with Wick limit are given in table 5.

Table 5 Comparison of calculated σ_{el} (0°) with Wick limit

sample	σ_{el} (0°) (b / sr)	Wick (0°) (b / sr)
U	15.50	14.74
Pb	13.59	13.68
Nb	7.22	6.76
Ni	3.56	3.24
Fe	3.29	2.80
Cr	2.89	2.56
Al	1.60	1.35

The comparison between the experimental[2~21] and calculated data of the angular distributions at small angles given by this work and others for ^{238}U, Pb, Nb, Ni, Fe, Cr and Al are shown in Fig. 3 and those between 0° and 180° are shown in Fig. 4. The calculated results using other global OMPs are shown in the figs. as well. The measured data of ^{238}U in the larger angle region come from Ref. [7], the inelastic cross sections with excitation up to 250 keV (corresponding to the experimental resolution of 250 keV) were included in the differential scattering cross sections. So the calculated data of ^{238}U include elastic scattering differential cross sections and the first two excited level inelastic cross sections and those of Al include both elastic scattering differential cross sections and the first excited level inelastic scattering differential cross sections. The solid lines represent calculated data of this work. The arrows are the Wick limit, in the figures, all of the scattering cross sections of the nuclei at zero degree of this work are larger or equal to the Wick limits, and this set of OMP can describe the angular distributions very well both in the small angle region and larger angle region. So the earlier global OMPs are improved at 14.8 MeV neutron energy for the mass number between 27 and 238.

ACKNOWLEDGEMENTS

We are very grateful to Dr. L. F. Hansen for providing us with the values of the differential elastic scattering cross sections of ^{238}U, Pb, Ni, Fe and Dr. Ma Gonggui for the values of ^{93}Nb. We would like to thank Chen Yingtang, Chen Zemin, Liu Yunchang, Wu Xuechao, Wang Wenhong, Zhang Jing, Chen Guojie, Chen Hongbin, they participated a part of experiment work. This work was supported in part by IAEA, the National Natural Science Fundation of China and China National Nuclear Industry Corporation.

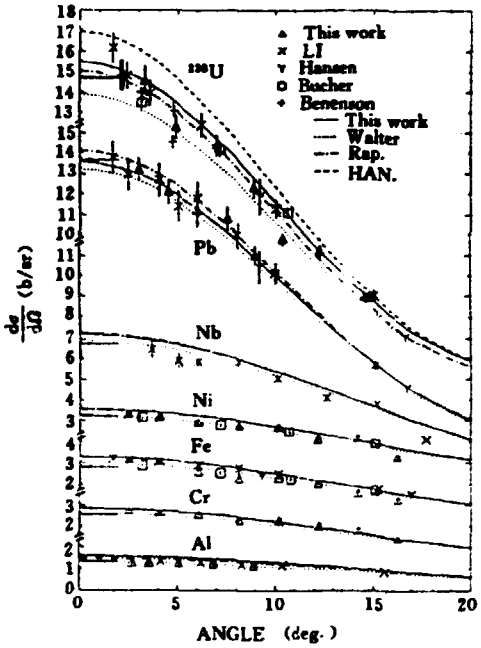

Fig. 3 Differential cross sections at small angles

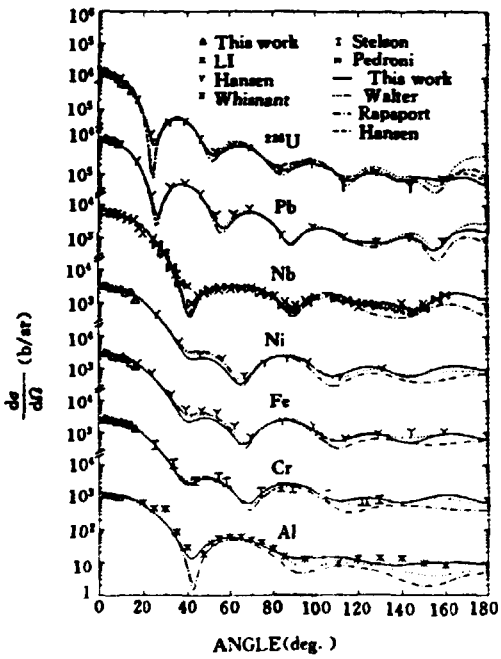

Fig. 4 Differential cross sections between 0° ~ 180°

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II THEORETICAL CALCULATION

A THEORETICAL CALCULATION OF n–T SCATTERING CROSS SECTIONS

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ABSTRACT

By using the phase shift analysis method, the σ_t, σ_{nn}, σ_{non} and $\sigma(0)$ of n–T scattering were calculated. The calculated results are in good agreement with the new experimental data and better than the previous calculations.

INTRODUCTION

In the previous evaluation of n–T neutron data[1], the compiled experimental values are adopted for σ_t and σ_{nn}, while the values calculated by the resonant group theory are adopted for σ_{non} and $\sigma(\theta)$ with ± 10% errors. The data about σ_t and σ_{nn} in the CENDL–2[2] have been improved. Especially, the cross sections in the range below 0.6 MeV are largely changed. Originally, the cross sections in the range $E_n < 0.6$ MeV reduced with the decreasing E_n. Now according to the Ref. [3] (1980), the values of σ_{nn} increase quickly with the decreasing E_n. The recommended values in the other ranges in the CENDL–2 are different from the previous recommendations, in which the largest change is 4%. For improving the calculated precision and fitting the new data of cross sections in the CENDL–2, it is necessary to calculate the cross sections again.

In this work, the cross sections σ_t, σ_{nn}, σ_{non} and $\sigma(\theta)$ were calculated by using the phase shift analysis method and the precisions of these cross sections are in the range of the experimental errors. The calculated values in the ranges $E_n <$ 0.6 MeV are in good agreement with the new experimental data. The calculated results for $\sigma(\theta)$ are also consistent with the experimental data and better than that from resonant group method, especially at the large angles.

1 THE CALCULATION METHOD

The formulas for calculating the cross sections are given in Ref. [4]. The dependences of the phase shifts on the neutron energy are

$$k^{2l+1} \operatorname{ctg} \delta_{lj} = A_{lj} + R^{l} k^2 + P_{lj} k^4 \tag{1}$$

where k is wave number of incident neutron, δ_{lj} the phase shift, A_{lj}, R_{lj} and P_{lj} are the adjustable parameters, and λ is the multiple number, $\lambda = 1$ (singlet state) or $\lambda = 3$ (triplet state), for n–T reaction, l is the quantum number of orbital angular momentum. In this work, three partial waves are taken into account, which means $l = 0, 1, 2$. A calculation on n–T scattering cross sections with phase shift analysis was also carried out by Carla et al.[5], but they didn't consider the absorptions and the results are only fitted to the ranges below the threshold energy (8.35 MeV). The results of σ_t calculated by Carla are also plotted in Fig. 1 for comparison.

Above 8.35 MeV (n,2n) channel is open, and beyond 11.32 MeV (n,3n) channel is also open. So the absorption factor y_{lj} must be introduced. When $y_{lj} = 1$, only elastic scattering channel is open, and $0 < y_{lj} < 1$ means nonelastic channel is open ($\sigma_{non} = \sigma_{n,2n} + \sigma_{n,3n}$, σ_{ny} is ignored). The dependences of y_{lj} on the incident neutron energies are

$$y_{lj} = \{ 1 + [(E_n - 8.35) (E_{lj} + G_{lj} E_n + H_{lj} E_n^2)^2] \}^{-1} \tag{2}$$

where the energies of incident neutrons are in MeV, F_{lj}, G_{lj} and H_{lj} are adjustable parameters. It is worth pointing out that because there are two open nonelastic channels, (n,2n) and (n,3n), in the ranges $E_n > 11.32$ MeV, we adopted different parameters in energy regions 8.35 MeV $< E_n <$ 11.3 MeV and $E_n > 11.3$ MeV for fitting the recommended experimental data very well.

We take simplex method[6], which is successfully used in the calculations of

n–D cross sections[7], for adjusting all parameters. The simplex method is a direct–search method with the function of multiple–demention and multiple–direction search. With the obtained parameters, the corresponding phase shift δ_{lj} and absorption factor y_{lj} can be obtained, and then the experimental cross sections can be reproduced very well by theoretical calculations.

2 CALCULATED RESULTS AND DISCUSSIONS

All parameters in different energy regions are given in tables 1~ 3. The comparison of the calculated cross sections σ_t, σ_{nn} and σ_{non} with the experimental data[2] are given in table 4. It can be seen that all calculated values are within the experimental errors. Figures 1 and 2 show the dependences of σ_t and σ_{non} on E_n respectively. The σ_t below 8.35 MeV given by Carla et al.[5] are also plotted. From Fig. 1 we can see our results are obviously better than that by Carla. In the regions below 0.6 MeV, our results can fit the new experimental data very well. Figures 3(a)~ 3(d) show the differential cross sections. The experimental data were taken from the work fulfilled by J. D. Seagrave et al.[8]. From these figures we can see that our results are better than that from the resonant group theory[1], especially at the large angles.

In general, our results calculated by phase shift analysis are better than that from other calculations, and in good agreement with the measured data.

Table 1 The parameters ($E_n < 8.35$ MeV)

L,λ	A	R	P
0,1	−0.19000	−0.76112	0.16779
1,1	0.13599×10^{-1}	0.29350	0.20778
2,1	5.1005×10	2.5033×10^{2}	-2.0070×10^{2}
0,3	−0.33649	2.3912	−4.5746
1,3	0.33035×10^{-1}	-0.46521×10^{-1}	0.95867
2,3	3.0616×10^{2}	-1.2512×10^{3}	4.4449

Table 2 The parameters ($8.35 < E_n < 11.3$ MeV)

L,λ	A	R	P	F	G	H
0,1	−1.1100	3.8214	−3.7847	-4.3932×10	7.9963	−0.36246
1,1	−0.37481	-1.2367×10^{2}	4.2566×10^{2}	−3.3679	0.7218	-0.36928×10^{-1}
2,1	−0.67026	3.9094	−3.4635	0.82059×10^{-2}	-0.11543×10^{-2}	0.12744×10^{-4}
0,3	−3.2362	2.5689×10	-4.9832×10	−6.4769	1.2945	-0.62054×10^{-1}
1,3	−0.19837	1.0328	−1.9935	0.36708	-0.85719×10^{-1}	0.49853×10^{-2}
2,3	1.7744×10	−6.5846	−6.3990	0.56936×10^{-4}	-0.57191×10^{-3}	0.86925×10^{-5}

Table 3 The parameters (E_n > 11.3 MeV)

L,λ	A	R	P	F	G	H
0,!	4.4085×10	2.4055×10^{2}	-9.7712×10	0.60233	0.13221×10^{-1}	-0.20844×10^{-2}
1,1	−0.39077	−0.17485	3.5087×10	0.15830×10^{-2}	0.45327×10^{-2}	-0.37182×10^{-3}
2,1	2.3022	-1.0172×10	1.2402×10	0.35345	-0.25912×10^{-1}	0.41009×10^{-3}
0,3	−0.45288	1.5762	−0.49711	0.52255×10^{-1}	0.42620×10^{-4}	-0.20899×10^{-3}
1,3	0.16323	−0.66487	1.4485	-0.40082×10^{-1}	0.24977×10^{-2}	-0.22912×10^{-4}
2,3	-1.6564×10	8.7660×10	-1.0048×10^{2}	−0.33203	0.42185×10^{-1}	-0.12808×10^{-2}

$[A] = (\mathrm{fm})^{-(2k+1)}$, $[R] = (\mathrm{fm})^{-(2k-1)}$, $[P] = (\mathrm{fm})^{-(2k-3)}$, $[G] = (\mathrm{MeV})^{-1}$, $[H] = (\mathrm{MeV})^{-2}$

Table 4 The comparison of the calculated cross sections with the experimental data

E_n (MeV)	σ_{ne} (mb)		σ_{nee} (mb)		σ_t (mb)	
	Th	Exp	Th	Exp	Th	Exp
1×10^{-11}	1703	1700 (30)	0.0	0.0	1703	1700 (30)
2.53×10^{-8}	1703	1700 (30)	0.0	0.0	1703	1700 (30)
0.1	1643	1650 (80)	0.0	0.0	1643	1650 (80)
0.3	1582	1610 (70)	0.0	0.0	1582	1610 (70)
0.5	1574	1570 (60)	0.0	0.0	1574	1570 (60)
1.0	1691	1700 (50)	0.0	0.0	1691	1700 (50)
1.5	1902	1895 (50)	0.0	0.0	1902	1895 (50)
2.0	2124	2120 (50)	0.0	0.0	2124	2120 (50)
3.5	2440	2435 (40)	0.0	0.0	2440	2435 (40)
4.0	2414	2410 (40)	0.0	0.0	2414	2410 (40)
5.0	2259	2240 (30)	0.0	0.0	2259	2240 (30)
6.0	2055	2030 (30)	0.0	0.0	2055	2030 (30)
7.0	1853	1815 (50)	0.0	0.0	1853	1815 (50)
8.5	1535	1528 (60)	6.2	6.5 (0.6)	1541	1535 (60)
9.5	1327	1360 (60)	35.1	35.3 (3.0)	1363	1395 (60)
10.4	1219	1240 (70)	49.0	48.7 (2.0)	1268	1289 (60)
11.5	1092	1118 (62)	52.1	52.5 (5.0)	1144	1170 (62)
13.0	1001	993 (70)	51.9	51.6 (5.0)	1053	1045 (33)
14.1	903	915 (70)	49.5	49.7 (5.0)	952	965 (14)
16.23	806	794 (70)	44.8	44.4 (5.0)	851	839 (49)
18.0	715	714 (65)	39.6	39.6 (5.0)	755	754 (51)
19.5	635	655 (60)	35.9	36.2 (5.0)	671	691 (50)
20.0	613	638 (60)	35.0	34.8 (4.0)	648	673 (50)

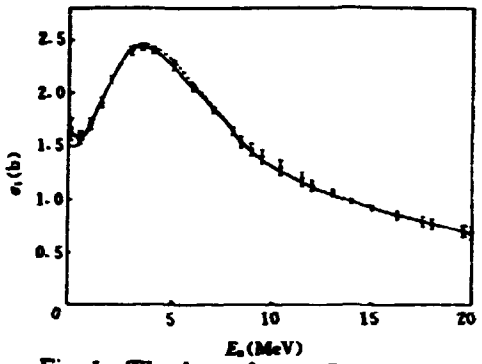

Fig. 1 The dependence of σ_t on E_n

— Present results, -- Carla's calculation, † Exp. data.

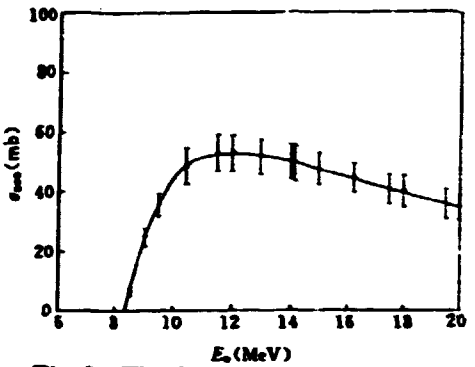

Fig. 2 The dependence of σ_t on E_n

— Present results, † Exp. data.

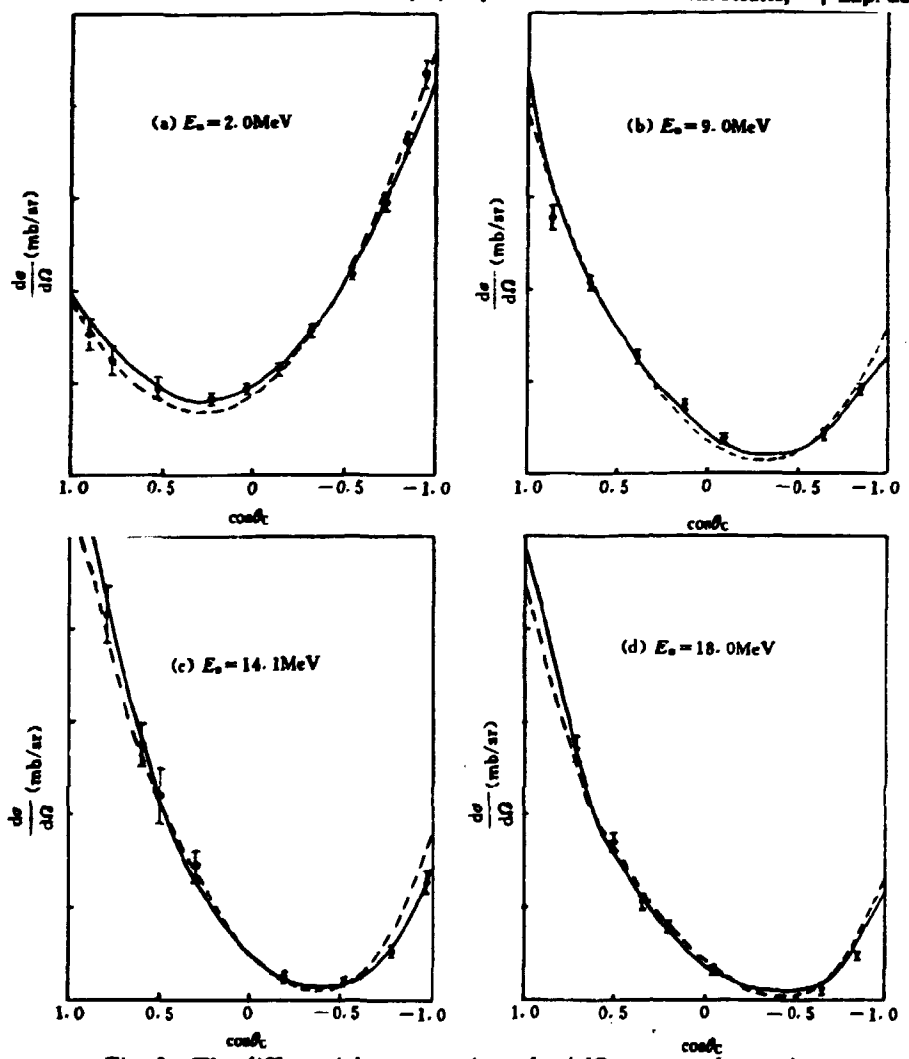

Fig. 3 The differential cross sections $d\sigma / d\Omega$ at several energies

—— Present results, - - - Resonant group theory, † Exp. data.

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THEORETICAL PROGRESS AT CNDC THEORY GROUP

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In 1992, CNDC theory group made progress in model study, code making and data calculations for low energy nuclear reaction, intermediate and high energy nuclear reaction. It also made progress in parameter library establishment. The following are the brief explanations.

I LOW ENERGY NUCLEAR REACTION

1 UNF code has been developed by combining the Hauser–Feshbach theory and Exciton Model. This code can be used for the calculations of double differential cross sections of neutron induced reactions below 20 MeV. In the code, the parity conservation and angular momentum conservation are taken into account in the exciton model, the pick–up mechanism for composite parti-

cle emissions and the recoil–nucleus effect are also taken into account. The discrete level effect in multi–particle emissions was included either.

2 By operating UNF code, (n,t) cross sections are calculated and fit the experimental data pretty well. UNF code is also used to calculate the double differential cross sections of α particle emission. The calculation is carried out for reaction $^{56}Fe(n,x\alpha)$ with incident neutron energy E_n = 14.5 MeV at θ = 30°, 45°, 90° and 135°. The calculations fit the experimental data nicely.

3 Based on MUP–2 code, MUP–3 code has been worked out. In MUP–3 the two time pre–equilibrium emissions, the refraction effect of incident particle on the nuclear surface are taken into account. This code not only can calculate data files 3, 4, 5, i. e, cross section, angle distribution and spectrum, but also can calculate data file 6, i. e, the nucleon double differential cross sections.

4 The direct inelastic scattering cross sections and angular distributions for the first excitation states of ^{56}Fe and ^{238}U at incident neutron energies 14.0 MeV and 20.0 MeV were calculated by coupled–channel optical model (CCOM) and DWBA method. The calculations show that the DWBA method is suitable for ^{56}Fe and the CCOM is suitable for ^{238}U. The inelastic scattering data calculated by DWBA method are always larger than those by coupled–channel theory, but the difference decreases as incident neutron energy increases.

5 In order to estimate the non–uniform effect of the single particle level density on particle–hole state density, a comparison is made by using the single particle level densities of harmonic oscillator potential and Fermi gas model. It is found that the non–uniform effect is stronger at low exciton states than at high exciton states. The calculations also show that the commonly used equidistant spacing model is a good approximation.

II INTERMEDIATE AND HIGH ENERGY REACTION

6 Cross sections for $p+^{241}Am$ reaction in 5.5~35 MeV energy region were calculated by CFUP1 code. Calculations for (p,F) and (p,2n) channels agree well with the experimental data between 8 MeV and 16 MeV. The calculations show that the nonelastic cross sections are mainly contributed from the fission cross section. When incident energy is larger than 15 MeV, the (p,pf) cross section has evident contribution. When incident energy is less than 20 MeV, neutrons are

the main emitted particles and when the incident energy is larger than 20 MeV, the light charged particle emission is important.

7 Using microscopic optical potential (MOP) with Skyrme force parameter, the excitation functions for p+^{89}Y reaction in $E<40$ MeV energy region are calculated. The comparisons with calculations of phenomenological optical potentials and with experimental data show that MOP is suitable for calculations of excitation function in proton induced reactions.

8 Based on Walecka's model and thermo field dynamics (TFD), the temperature dependent relativistic microscopic optical potential for nuclear matter is obtained in which the polarization and correlation contributions is taken into account. The Schrodinger equivalent potential and mean free path for nuclear matter are also obtained. With local density approximation, the same quantities are obtained for finite nuclei. The results are reasonable for single particle energies between $\approx$ 40 MeV and 1000 MeV relative to the Fermi energy.

9 Based on the available experimental data of ^{63}Cu and its neighbor nuclides ^{62}Ni and ^{64}Zn, a set of proton optical potential parameters for $E_p<55$ MeV is obtained. Through adjusting neutron and other charged particle optical potential, level density parameters as well as exciton model parameter K, all cross sections for reaction p + ^{63}Cu are obtained in energy region 3~ 55 MeV. The calculations agree well with experimental data for reactions (p,p'), (p,n), (p,3n) and (p,np+d), but for reactions (p,2n) and (p,2nd+p3n+nt) further study is needed.

10 In order to generalize the exciton model to high energy nucleon–nucleus scattering, an empirical formula of relativistic exciton transition rate is given by taking account of the relativistic effect. This formula is suitable for atomic number from 40 to 252 and for incident nucleon energy from 40 to 1040 MeV.

11 An attempt of applying QNCD (quantum nucleon cluster dynamics) or QMD (quantum molecular dynamics) to calculate nuclear data for intermediate and high energy is undertaking. It can be expected that the nucleons or light particles are released from the highly excited nucleus during its time–space evolution. A code has been made based on QNCD and applied to study the thermalization in 830 MeV p+Fe reaction. It is found that the thermalization is reached in a tube–like volume along incident direction, i. e, a local thermalization rather the thermalization of the whole nucleus.

III PARAMETER LIBRARY ESTABLISHMENT

12 For the practical and convenient use, the Chinese Evaluated Nuclear Parameter Library (CENPL) is under established, CENPL contains six sub-libraries, each of them consists of two parts, the data files and the management-retrieval code system. The data files store evaluated basic nuclear constants and model parameters. The management-retrieval codes are used to retrieve relative information of parameters.

The six sub-libraries are

(1) Atomic masses and characteristic constants for nuclear ground state (MCC). So far the atomic masses of 4760 nuclides, half-lives or abundances, spin and parities for nuclear ground state have been put into the data file and the retrieval code for single nucleus (SN) is made out.

(2) Discrete level schemes and branch ratio of γ decay (DLD).

(3) Level density parameters (LDL). The data file which contains relative experimental data (LRD) and level density parameters (LDP) is made out. Its retrieval code for SN has been set up.

(4) Giant dipole resonance parameters for γ-ray strength function (GDR). At present, experimental data of 102 nuclides have been put in the data file and the management-retrieval code system is established.

(5) Fission barrier parameters (FBP). The data file, including the parameters recommended by Lynn, Back-Britt and Ohsawa, and the management-retrieval code system have been set up.

(6) Optical model parameters (OMP).

IV OTHERS

13 Besides the influence of nuclear deformation fluctuation on particle emission has been studied, the influence of temperature at each local equilibrium stage with exciton number n on the particle emission is also studied. It is found that the temperature of the thermal bath provided by different local equilibrium stage of exciton number n taking as a constant as $kT = (E/a)^{1/2}$ is just reasonable and suitable.

14 To explain the double-slope behavior of $\ln < Fi > \sim -\ln\delta y$ drawings in particle production in high energy hadronic interactions and heavy ion collisions, the weighted distribution in particle production is proposed. The second slope is due to the random cascade process, while the first one is mainly due to the unflat of the average distribution.

THE FORBIDDEN ANGULAR REGION OF SECONDARY PARTICLE EMISSION IN THE LABORATORY SYSTEM

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The calculated double differential cross sections (DDX) can be represented by Legendre coefficients (L.C.) in the center of mass system (C.M.S.). From the point of view of nuclear engineering calculation, it is more convenient to use DDX represented in laboratory system (L.S.). For DDX, it holds that

$$\frac{d^2\sigma}{d\varepsilon_L d\Omega_L} d\varepsilon_L d\Omega_L = \frac{d^2\sigma}{d\varepsilon_C d\Omega_C} d\varepsilon_C d\Omega_C \tag{1}$$

where the quantities with subscript "L" and "C" mean in L.S. and in C.M.S., respectively. The Jacobian is given by

$$d\varepsilon_C d\Omega_C = \sqrt{\frac{\varepsilon_L}{\varepsilon_C}} d\varepsilon_L d\Omega_L \tag{2}$$

If the double differential cross sections are represented by L.C., we have

$$\frac{d^2\sigma}{d\varepsilon_L d\Omega_L} = \sum_l \frac{2l+1}{4\pi} F_l(\varepsilon) P_l(\cos\theta_L) \qquad \text{in L.S.} \tag{3.1}$$

$$\frac{d^2\sigma}{d\varepsilon_C d\Omega_C} = \sum_l \frac{2l+1}{4\pi} f_l(\varepsilon) P_l(\cos\theta_C) \qquad \text{in C.M.S.} \tag{3.2}$$

The relation of the Legendre coefficients between L. S. and C. M. S. is given by

$$F_k(\varepsilon_L) = \frac{1}{2} \sum_l (2l+1) \int f_l(\varepsilon_C) \sqrt{\frac{\varepsilon_L}{\varepsilon_C}} P_l(\cos\theta_C) P_k(\cos\theta_L) d\cos\theta_L . \tag{4}$$

with

$$\varepsilon_C = \varepsilon_L(1 + \beta^2 - 2\beta\ \cos\theta_L) \tag{5}$$

$$\cos\theta_C = (\ \cos\theta_L - \beta) / \sqrt{1 + \beta^2 - 2\beta\ \cos\theta_L} \tag{6}$$

$$\beta = \frac{\sqrt{m_a m_b}}{M_C}\sqrt{\frac{E_L}{\varepsilon_L}} \tag{7}$$

where E_L denotes incident particle energy in L.S.; m_a and m_b are the masses of incident and outgoing particles respectively, and M_C is the mass of the compound nucleus.

Using L. C. to calculate the DDX in L. S., one has to pay attention to the forbidden angular region for a certain outgoing energy because of the motion of the center of the mass. In general the outgoing energies in C. M. S. satisfy

$$\varepsilon^C_{min} \leqslant \varepsilon_C \leqslant \varepsilon^C_{max} \tag{8}$$

$$\varepsilon^C_{min} = 0 \quad \text{for} \quad \text{neutron}$$

Let us denote

$$D = \frac{\sqrt{m_a m_b}}{M_C}\sqrt{E_L} = \beta\sqrt{\varepsilon_L} \tag{9}$$

For charged outgoing particle, the forbidden angular region in three cases can be obtained as follows:

(1) The allowed outgoing angular region is given by

$$-1 \leqslant \cos\theta_L \leqslant \frac{(\varepsilon_L + D^2 - \varepsilon^C_{min})}{2D\sqrt{\varepsilon_L}} \tag{10}$$

if

$$(\sqrt{\varepsilon^C_{min}} - D)^2 \leqslant \varepsilon_L \leqslant (\sqrt{\varepsilon^C_{min}} + D)^2 \tag{11}$$

(2) There is no forbidden angular region, that is, the allowed angular region is

$$-1 \leqslant \cos\theta_L \leqslant 1 \tag{12}$$

if

$$(\sqrt{\varepsilon^{C}_{min}} + D)^2 \leqslant \varepsilon_L \leqslant (\sqrt{\varepsilon^{C}_{max}} - D)^2 \tag{13}$$

(3) The allowed outgoing angular region is given by

$$\frac{(\varepsilon_L + D^2 - \varepsilon^{C}_{max})}{2D\sqrt{\varepsilon_L}} \leqslant \cos\theta_L \leqslant 1 \tag{14}$$

if

$$(\sqrt{\varepsilon^{C}_{max}} - D)^2 \leqslant \varepsilon_L \leqslant (\sqrt{\varepsilon^{C}_{max}} + D)^2 \tag{15}$$

In the case of neutron emission only Eqs. (14) and (15) are needed to determine the allowed angular region. As an example, the spectrum and allowed angular region of DDX for α particle emission in reaction ^{56}Fe(n,α) at E_n = 14.5 MeV are shown in table 1.

The forbidden angular region must exist if the L. C. are given in L. S.. For high outgoing energies the forbidden region is in large angles area, while for low outgoing energies of charged particles the forbidden region is in small angles area.

In the ENDF / B–6 format for representation of file 6, if L. C. in L. S. is used, the negative values of DDX in the forbidden angular region could occur. The phenomena of negative values of DDX could be avoided if tabulated DDX are given or isotropic distribution is assumed. But the former could produce a huge evaluated data file and the latter could be unreasonable physically. Yet using L. C. in C. M. S. to represent the DDX also can avoid the phenomena of negative values of DDX, but it would be difficult to users for transforming the DDX from C. M. S. into L. S..

In conclusion, in the case of using L. C. in L. S. to represent DDX in ENDF / B–6 format, having a "flag" to denote the forbidden angular region seems to be necessary.

Table 1 Spectrum of outgoing α and allowed angular regions in $^{56}Fe(n,\alpha)$ reaction with E_n = 14.5 MeV

ε_α (MeV)	Spectrum	$\{\cos\theta_L\}_{min}$	$\{\cos\theta_L\}_{max}$
3.93	0.000		
4.12	0.00002	−1.000	−0.664
4.29	0.00007	−1.000	−0.331
4.48	0.00019	−1.000	−0.002
4.67	0.00048	−1.000	0.324
4.86	0.0012	−1.000	0.646
5.06	0.0028	−1.000	0.965
5.27	0.0062	−1.000	1.000
5.70	0.0366	−1.000	1.000
6.15	0.101	−1.000	1.000
6.82	0.186	−1.000	1.000
7.12	0.253	−1.000	1.000
7.64	0.282	−1.000	1.000
8.19	0.273	−1.000	1.000
8.75	0.235	−1.000	1.000
9.34	0.210	−1.000	1.000
9.96	0.160	−1.000	1.000
10.27	0.137	−0.862	1.000
10.59	0.111	−0.472	1.000
10.92	0.0843	−0.097	1.000
11.25	0.0599	0.273	1.000
11.59	0.0381	0.639	1.000
11.92	0.000	0.000	

CMUP2 – A PROGRAM FOR CALCULATING NEUTRON OR CHARGED PARTICLE INDUCED REACTIONS IN ENERGY RANGE UP TO 50 MeV

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CMUP2 is a program for calculating the neutron or charged particles (p, d, t, ^{3}He, α) induced reactions on medium–heavy nuclei in the incident energy range of 1 ~ 50 MeV. This program was written in FORTRAN–77 on computer M–340S and also has a version on computer MICRO–VAX–II.

CMUP2 is constructed within the framework of the optical model, the preequilibrium (PE) statistical theory based on exciton model, and the evaporation model. In the first, second, and third particle emission processes, preequilibrium emission and evaporation are considered; in the fourth particle emitting process, only evaporation is considered.

The multi–particle and –hole state density with considering the Pauli exclusion principle is used in the exciton model[1~4].

For composite particle emission, the pick–up mechanism of cluster formation[5~7] was used in the first, second, and third particle emission processes. The Gilbert–Cameron level density formula[8] was applied in program CMUP2. The inverse cross sections of the emitted particles used in statistical theory are calculated from the optical model. The partial widths for γ–ray emission are calculated based on the giant dipole resonance model with two resonance peaks.

In the optical model calculation, the Becchetti and Greenlees's[9] phenomenological optical potential is adopted, as usual which parameters are given by a program for automatically searching for the optimum optical model parameters. Besides, CMUP2 can also do microscopic optical potential calculations based on Skyrme force[10] and phenomenological optical potential calculation by Varner et al.[11] for n and p channels. Neumanove method

is used to solve the radial equation in optical model, with step length 0.1 fm, step number 150 and maximum number of fractional waves 60. Coulomb wave functions used in optical model are calculated by the continued fraction method[12]. The calculated direct reaction and compound nucleus elastic scattering results obtained with other codes can be added by the input data of the program CMUP2.

In the energy range up to 50 MeV, CMUP2 can give the calculated results for optical model quantities and all kinds of cross sections in first, second, third, and fourth particle emission processes. When the incident energy is near to 50 MeV, the fourth particle emission process includes the contributions from the fifth particle emission process for heavier nuclei. CMUP2 also gives energy spectra of all emitted particles in first and second particle emission processes.

The output data of CMUP2 include : total and shape elastic scattering cross sections (only for neutron as projectile); total cross section; radiative capture cross section; (x, x'), (x, x_1x_2), and $(x, x_1x_2x_3)$ reaction cross sections, where x', x_1, x_2, and x_3 could be n, p, t, ^{3}He, d, or α; $(x, x_1x_2x_3x_4)$ reaction cross sections, where x_1 and x_2 could be n, p, t, ^{3}He, d, or α, but x_3 and x_4 could only be n or p; the elastic scattering angular distribution and the ratio of the elastic scattering differential cross section to the Rutherford differential cross section; the energy spectra of x' particle in (x, x') reaction and of x_1 and x_2 particles in (x, x_1x_2) reaction.

In order to make comparison with experimental data conveniently, the sum of cross sections of all reactions which lead to the same residual nucleus is also given, for example, $\sigma_{x,2np}+\sigma_{x,nd}+\sigma_{x,t}$. We call them residual nucleus yield cross sections.

In program CMUP2, we give the emission cross section of particle y in reaction (x, yx') in one– and two–particle emission processes without regard to what particle x' is and the corresponding energy spectra of particle y in reaction (x, yx'), where y can be n, p, t, ^{3}He, d, or α.

CMUP2 has been already used to calculate reactions of : p+^{89}Y, p+^{63}Cu, n+^{56}Fe. Pretty good results in agreement with the experimental data were obtained. The application practices show that CMUP2 is a useful and convenient program for users.

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CFUP1 – A PROGRAM FOR CALCULATING NEUTRON OR CHARGED PARTICLE INDUCED REACTIONS ON FISSILE NUCLEI IN ENERGY RANGE UP TO 35 MeV

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CFUP1 is a program for calculating the neutron or charged particles (p, d, t, ^{3}He, α) induced reactions on fissile nuclei in the incident energy range of 1~35 MeV. This program is written in FORTRAN-77 on computer M-340S and also has a version on computer MICRO-VAX-II.

The theories and calculated methods used in CFUP1 are similar with CMUP2[1], except for including fission channels.

In the evaporation model, the fission probability of the compound nucleus is calculated by the effective single peak fission barrier formula. The formula of level density on saddle point is taken from Ref. [2]. The ν value of the fission process is calculated by Howerton's semi-classical formula[3].

In the energy range of 1~35 MeV, CFUP1 can give the calculated results for optical model quantities and cross sections in first, second, third, fourth, and fifth particle emission processes as well as secondary particle and fission neutron energy spectra.

The output data of CFUP1 include :

1 The cross sections and ν values :

σ_{tot} (only for neutron as projectile), σ_{el} (only for neutron as projectile),

σ_{non} , $\sigma_{x,\gamma}$, $\sigma_{x,n}$, $\sigma_{x,2n}$, $\sigma_{x,3n}$, $\sigma_{x,4n}$, $\sigma_{x,5n}$, $\sigma_{x,np}$, $\sigma_{x,p}$,

$\sigma_{x,d}$, $\sigma_{x,t}$, $\sigma_{x,^3He}$, $\sigma_{x,\alpha}$, $\sigma_{x,f}$, $\sigma_{x,n'f}$, $\sigma_{x,2nf}$, $\sigma_{x,3nf}$, $\sigma_{x,4nf}$,

$\sigma_{x,pf}$, $\sigma_{x,F}$ (total fission cross sections).

ν values of various fission processes.

2 The elastic scattering angular distributions and the ratios of the elastic scattering differential cross section to Rutherford scattering differential cross section.

3 The energy spectra of all secondary particle in one- to five-particle emission processes and the fission neutron spectra of various fission processes.

CFUP1 has been already used to calculate several reactions of p+^{235}U, p+^{241}Am, n+^{240}Pu. Pretty good results in agreement with the experimental data were obtained. Application practices show that CFUP1 is a useful and convenient program for user.

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DIFFUSION PROCESS OF NUCLEAR FISSION

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In the calculations of fission width and fission cross section, the Bohr–Wheeler formula[1] is generally used. This formula is derived based on Bohr channel theory in which it is assumed that the nucleus has reached its statistical equilibrium both at the ground state and the fission state (generally, the saddle point is taken as the fission state). The particle emissions occur at its ground state whenever the excitation energy is large than the particle binding energy. While the nuclear fission occurs at its saddle point whenever the excitation energy is large than the height of fission potential. In the theory, the detail of the process for the nucleus deforming from its ground to the saddle point is not taken into account, the process is simply treated as a sudden finished process, no time is needed, no particle emission occurs in the process. This theory has been widely used and works well for low energy reactions. But in recent years, when this theory is applied to heavy ion collisions with higher incident energy, it is found that this theory can not explain the experimental data well. Such as in reaction $^{16}O + ^{142}Nd \rightarrow ^{158}Er$ at incident energy 207 MeV, the measured neutron multiplicity is 4.2[2], while the calculation value by this theory is only 1.6, much lower than the measured value.

In order to explain the experimental data for high energy heavy ion collisions, a fission diffusion model was proposed[3]. This model takes the fission process as a diffusion process: the nucleus, under the action of fission potential, is expressed by probability in the deformation space. The probability diffuses from the ground state to saddle point and to scission point. The total probability on the left side of the saddle point are the probability characterizing the existence of the nucleus and the probability on the right side of the saddle point are the fission probability. The nucleus has large friction constant compared to the oscillation frequency in the potential well, i.e. the nuclear deformation is a slow oscillating process compared to the damping process, the oscillation period is much longer than the decay length of the damping process. This diffusion process can be described by Smoluchowski equation[4]. Besides, during the diffusion process, the nucleus can release light particles such as neutron, proton and alpha particle. For taking light particle emission into account, the extensive

Smoluchowski equation was proposed[3]:

$$\frac{\partial P(x,t)}{\partial t} = \theta \frac{\partial}{\partial x}\left(\frac{\partial U}{\partial x}P(x,t) + \frac{\partial P(x,t)}{\partial x}\right) - \sum_{i=n,p,\alpha} \lambda_i P(x,t)$$

where $P(x,t)$ is the probability of the nucleus at deformation x and time t. $U(x)$ is the dimensionless fission potential. The dependence of the nucleus on friction constant and temperature is involved in θ. The first term on the right side describes the diffusion while the second term stands for the particle emissions. λ is the particle decay rate.

As general, the saddle point is taken as the fission point, i. e. if the probability flow goes over the saddle point, the fission occurs. The total probability of the nucleus, $\pi(t)$, is the integral of $P(x,t)$ on the left side of the saddle point. The probability flow, $J(t)$, at the saddle point is the time differential of $\pi(t)$. The fission rate can then be defined as $\lambda_f(t) = J(t) / \pi(t)$. Its behavior is shown in Fig. 1. At the very beginning, the fission rate is very small, this is because the amount of probability flow reaching to the saddle point is very small. Afterwards, the fission rate goes up steadily, over a peak, and at last reaches to a constant value which is the result of Bohr channel theory.

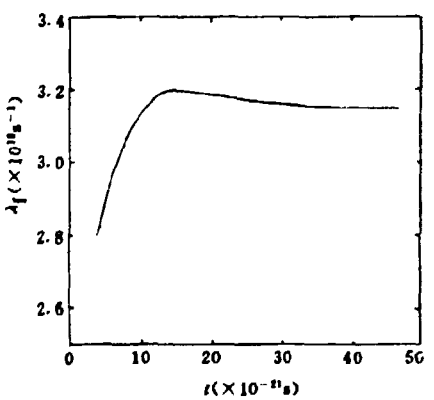

Fig. 1 Fission rate versus time for composite nucleus ^{240}Pu at T = 2 MeV

Process before reaching to the constant value is called "transient process". This is the essential process of the fission diffusion model. In the process, the

fission rate is smaller than that in Bohr channel theory except near the peak. (The peak is called "overshooting", it has no physical importance, because its existence depends on the choice of fission point. It shows up only when taking the fission point near the saddle point. When points beyond the saddle point are taken as the fission point, the peak soon disappears. The physical fission point is the scission point rather than the saddle point). It is the existence of transient process that leads to the enhancement of light particle emission prior to fission. Especially in heavy ion collisions with higher incident energy, the nucleus has higher excitation energy, the particle emission rates are high, the nucleus soon decays through emitting light particles before the fission rate reaches its constant value. That is why the Bohr channel theory can work well for low energy nuclear reactions, but for high energy heavy ion collisions, it does not work well, the transient process is important and the fission diffusion model must be used. This model has been applied to explain the enhancement of neutron emission in heavy ion collisions forming the composite nucleus ^{158}Er. The experimental data are well reproduced by the model calculations[5, 6].

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REVIEW AND EVALUATION OF FISSION BARRIER PROPERTIES RESEARCH

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ABSTRACT

The situation of researching nuclear fission barrier properties is introduced and reviewed briefly, especially reviewed and evaluated on the nuclear fission barrier parameters obtained from Refs. [1～6] for nuclear parameters library constructed.

INTRODUCTION

The situation of researching nuclear fission barrier properties is introduced and reviewed briefly in the present paper. The quantitative combination of macroscopic and microscopic theoretical methods of liquid drop model and potential energy surface calculation in a deformed shell model field are reviewed. For example, the set of calculations for $76 < Z < 100$, $140 < N < 184$ given by W. M. Howard and P. Moller[1] provides a way to study nuclear fission barrier properties from the theoretical point of view. The other way is to measure some physical quantities, then from the quantitative analysis of the relation between those quantities and fission barrier to determine the fission barrier parameters, such as, ground state spontaneous fission half lives measurement and analysis; fission isomers and intermediate state measurement and analysis; excitation function measurement and analysis; fission probability measurement and analysis of (d,pf), (t,pf), (^{3}He,αf), (p,p'f), (t,t'f) ··· by using direct reaction induced fission in the region of excitation energy below neutron binding energy and so on[2～6]. A main review on the theoretical analysis and calculations of Refs. [1～6] is presented. The nuclear fission barrier parameters and the levels at saddle point obtained from Refs. [1～6] are evaluated for nuclear parameters library of CNDC constructed, and described in Sec. 2.

REVIEW AND EVALUATION

W. M. Howard and P. Moller presented the results of calculated fission barriers and others for nuclei with $76<Z<100$ and $140<N<184$ in Ref. [1]. In this work a macroscopic droplet model with 1973 sets of parameters and a microscopic modified oscillator model for shell correction calculation as a function of elongative, necking, mass-asymmetric, axially asymmetric shape coordinates are used. It is claimed that the parameters of 1125 nuclides obtained are good enough for the application using in the fields of fission cross section calculations, r-process path calculation in Astrophysics, Cosmophysics and radioactive waste treatment calculations and so on. It is clear that the range of nuclides is more wide, not only for actinide nuclides, but also for the others. The calculated results for actinides is in good agreement with Refs. [7~8]. The theoretical calculations by means of quantitative combination of macroscopic and microscopic method are certianly available for those nuclei having no any experimental information. The calculated maximum fission barrier heights for Th-Cf elements are shown in Fig. 1 by + signs.

J. E. Lynn calculated n + actinides cross section up to 3 MeV presented in Ref. [2]. In the calculation Hauser-Feshbach formula neglecting direct, semi-direct and pre-equilibrium mechanism, constant temperature level density with modification for low excitation at saddle point and double-humped barrier with complete damping model in second well for fission transmission coefficient calculation were adopted. The values of barrier parameters from the analysis of fission data on actinide nuclei were recommended and shown in Fig. 1 by small squares signs. It is the one of main conclusions of the work that the level density at the first barrier is 3~5 times greater than the level density associated normal deformation, but there is not such a great different at the outer barrier.

Using double-hamped barrier T. Ohsawa[3] simplified complete damping model and calculated fission cross section and recommended barrier parameters for 24 nuclei from ^{232}Pa to ^{253}Cf. In the calculation level density at saddle point were considered with collective enhancement effect. T. Ohsawa's results are similar to the one given by J. E. Lynn for the first barrier E_A, but there are some difference for the second barrier E_B of heavier nuclei A_m, C_m, C_f, B_k. The results of Ref. [3] are shown in Fig. 1 by inverse triangles.

B. B. Back et al. measured the fission probability distribution of (d,pf), (t,pf), (α,αf), (t,t'f), (p,p'f), (^{3}He,df), (^{3}He,αf) reactions induced by direct reaction mechanism for doubly even actinide nuclei of ^{230,232,234}Th, ^{232,236,238,240}U, ^{238,242,244}Pu and ^{244,248,250}Cm, which were analyzed by a statistical model involving resonant penetration of the double-humped fission barrier[4]; for

odd A and doubly odd actinide nuclei of $^{219,231}Th$, $^{231,232,233}Pa$, ^{239}Np, ^{241}Pu, $^{240,241,243,245,247}Am$, ^{249}Cm, ^{249}Bk, which were analyzed by a satistical model of complete damping in the second well of the fission barrier[5]. The height of the double-humped fission barrier are shown in Fig. 1 by dotted signs.

Ref. [6] presented the systematic calculations for U, Pu elements in energy range between 3 to 20 MeV by a combination of optical model, evaporation model, exciton model. In the calculations, effective single barrier and a modified Fermi gas model by a enhancement factor for level density at saddle point was used. According to the experimental fission cross section data, the fission barrier parameters and enhanced level density factors at saddle point were obtained. The heights of the effective single barriers are shown in Fig. 1 by cross signs. It was concluded that the enhancement factors of level density at saddle point compared with it normal deformed states were 1.25~ 1.79 for doubly even U, Pu elements, 4.25~ 4.85 for odd A U, Pu elements. Compared the enhancement factor given in Ref. [6] with the one given by J. E. Lynn in Ref. [2] in the same energy range of 3~4 MeV, a fairly good agreement was obtained.

All of the heights of fission barrier for Th-Cf elements presented by Refs. [1~6] obtained in different ways as mentioned in above are plotted in Fig. 1. It is worth to pay attention to the following : (1) The most remarkable feature of those heights of fission barrier obtained from Ref. [1~6] is that E_A are at 4.5 ~6.8 MeV over the entire region from Th through Cf and E_B steady decreases of from 6.3 MeV in Th to about 4 MeV for Cm isotopes except the results of Ref. [1] for Th. (2) There are some apparent odd-even fluctuations in E_A and E_B for each different way to obtian the data, for example, in E_A for U, Pu and Am elements presented by Ref. [4, 5], in E_B for Am elements presented by Ref. [9]. (3) The results presented by Ref. [1] are systematically lower than the others for Np, Pu, Am, Cm, Bk and Cf elements, but higher than the others for Pa and some lighter U elements, and it is about 2 MeV lower than the others for Th elements. The apparent discrepancy means that there still remains something not understood from the theoretical calculations. Maybe more complicated asymmetric shape should be taken into account in such a kind of theoretical calculations.

The another important point is about the levels at saddle point. From the analysis of the calculations of Refs. [2~6], the barrier spectra for fission calculation for doubly even actinide nuclei employed by J. E. Lynn, and on even Z odd N or odd Z even N fissioning nucleus obtained from the Bolsterli et al.'s calculations employed by Ref. [5] could be generalized to use. In the continuous energy range of saddle point levels, the constant temperature formula is adopted in Ref. [2], the Girbert-Cameron formula of Fermi gas

model is adopted in Ref. [6]. In any event, it can be concluded that the level density at siddle point is enhanced compared with it at the normal deformation by a appropriate collective enhancement factors corresponding to the large deformed nuclear shape. According to Refs. [2, 6] it seems that the empirical maximum enhancement factor of level density at saddle point could be about 4 in general terms.

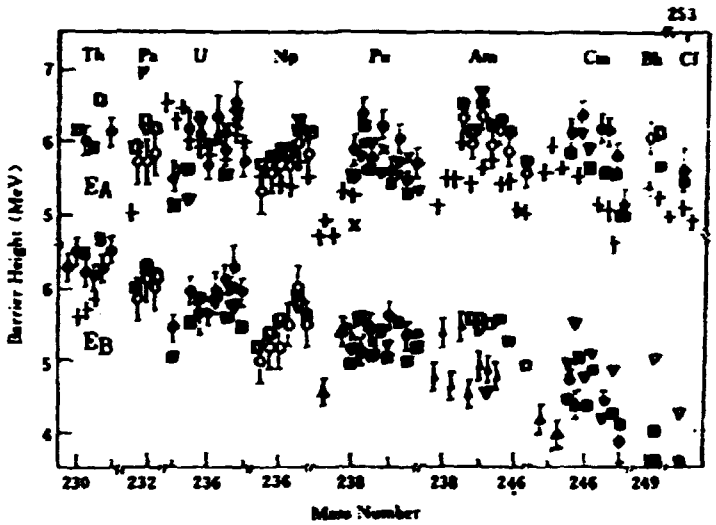

Fig. 1 Barrier height of Refs. [2~6, 9]

● ○ B. B. Back et al., ■ □ J. E. Lynn, ▲ △ H. C. Britt et al.,

▼ ▽ T. Ohsawa, × Zhang and Wang, + W. M. Howard and P. Moller

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III DATA EVALUATION

TECHNIQUES USED FOR CHARGED PARTICLE NUCLEAR DATA EVALUATION AT CNDC

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ABSTRACT

The methods and techniques used for Charged Particle Nuclear Data (CPND) evaluation at Chinese Nuclear Data Center (CNDC) are summarized in this report, including compilation and evaluation of experimental data, nuclear reaction theory and model calculation, systematics research and comprehensive recommendation etc..

INTRODUCTION

Charged Particle Nuclear Data (CPND) have been widely used in basic scientific researches on nuclear force, nuclear structure, nuclear reaction mechanism and nuclear astrophysics etc.; also used in engineering and technology such as space radiation effects, neutron sources, biomedical isotope production, radiation therapy, activation analyses, radiation processing, accelerator shielding and fusion reactor designs.

Due to Coulomb repulsion between incident charged particle and target nucleus, the cross sections of charged particle nuclear reaction are much smaller than those of neutron, they are in about millibarn region; besides, there is a Coulomb threshold, which is dependent upon Coulomb barrier, when incident charged particle energy is less than the Coulomb threshold, the nuclear reaction can not be induced, even if reaction energy $Q>0$. But in general, the threshold for a reaction of $Q>0$ equals to zero. These are the two characters of charged particle nuclear reaction.

Compared with neutron experimental data, CPND are scarce and existing data are scattered, usually the measured data are not enough to do an

evaluation. Therefore, Chinese Nuclear Data Center (CNDC) puts the stress on the establishment of nuclear reaction theory and model calculation codes for CPND.

By the end of fifties, the measurements of CPND with light particle incident were started in China Institute of Atomic Energy. About ten years later, the studies of nuclear reactions induced by heavy ion have been performed. From 1975 on, the evaluations[1] of CPND on light, intermediate, heavy and fissionable nuclides have been carried out at CNDC in the energy region from threshold to 20 MeV or above.

In general, data are generated from experiment, theory and systematics. The experiment is the first and direct source, and the base of both the latters.

The main task of evaluators consists in the collection, comparison, critical assessment and selection of experimental data and associated covariances; nuclear model calculations and systematics must be used to fill gaps and remove inconsistencies in the available experimental data; followed by the derivation of preferred values by appropriate combination procedures, or self-consistent sets of those if necessary.

1 EVALUATION OF EXPERIMENTAL DATA

1.1 Compilation and Collection of CPND

The measured data need to be compiled in EXFOR format for preserving, exchanging and using. CNDC has compiled the CPND measured in China, and sent to NDS / IAEA.

It is high important to make full use of all the available information on nuclear data. This is one of cardinal principles of nuclear data evaluation; because the more information is utilized, the more reliable and accurate recommendation is obtained. Therefore the related experimental data must be collected as complete as possible.

The bibliographies and indexes to CPND used at CNDC are as follows :

Nuclear Science Abstracts; Nuclear Data Table; Atomic Data and Nuclear Data Table; INIS Atomindex; USRL-50400, BNL-NCS-50640, BNL-NCS-51771; CPND EXFOR Master-File Index.

The numeral data can be got from EXFOR entries, some papers and their authors sometimes; however, it is necessary for this purpose to read graph, because parts of the experimental data have not been compiled in EXFOR entries yet. A part of numeral data used for CPND evaluation at CNDC were taken from the figures of related articles and reports. The error of reading graph is

about 1~5%.

1.2 Comparison and Evaluation of CPND

The first step, experimental data are analysed on the basis of measuring method and instrument, correction factors and covariance matrixes etc.

The main methods used in measurements of CPND are as follows :

(1) Measurement of outgoing particles : "$E/\Delta E$" and "E/t" measurements, magnetic deflection, mass-separator, pulse-height discrimination;

(2) Measurement of production nucleus : activation, chemical separation, collection of recoil nucleus, and their combination.

In a complex reaction, the method with particle identification is better than the others, and the more the instrumental resolution is high, the more the measured result is accurate.

In absolute determination, the incident charged particle flux is often measured by beam current integration. The unstability of beam current integrator is one of important sources for data difference sometimes, because there are usually some interferences in experiment, if they are not noticed and eliminated. In addition, the background due to big elastic scattering is also a factor not to be ignored.

In relative measurement, if the standard data of monitor are renewed, the result should be renormalized.

When any correction and covariance in evaluated experiments are unreasonable or omitted, we adjust or supplement them, if possible; otherwise, such experimental data shouldn't be adopted.

After this process, available experimental data have been selected.

The second step, all chosen data are plotted in different figures according to data categories respectively, in order to compare each other. If the discrepancy among them is large, a further and refined analysis is needed to decide which should be accepted or rejected. If it is difficult to do this, the basic principle is that the minority is subordinate to the majority, or equal-weight average can be adopted.

Currently, simultaneous evaluation is proposed and applied to estimate cross sections, especially for important ones. It is advanced in comparison with individual evaluation usually adopted in many works because of the following reasons. In the former method, it can be expected to reduce contribution of systematic errors in experiments to uncertainties of evaluated results, and original values of experimental data are used without renormalizing even ratio data.

Simultaneous evaluation method has been used in neutron data evaluation at CNDC. It will be utilized for evaluating CPND.

1.3 Data Processing

The data fit programs with Legendre polynomials[2] for angular distribution, orthogonal polynomials[3] and spline functions[4] with knot optimization are used at CNDC. Both the latters can estimate not only the evaluated cross sections but also the covariances associated with them. The both quantities can be estimated taking account of correlation on the cross section measurements.

Model theory is also used to fit experimental data[5], as shown in Fig. 1. Sometimes, eye–guide is convenient and useful for this purpose.

Because of large systematic errors and discrepancies between different experimental results which in many cases are very difficult to disclose and eliminate, or lack of experiment data, the further and more precise measurement is necessary, if possible.

If evaluated experimental data are not quite enough for application requirement, theoretical model calculation, systemstics research or comprehensive recommendation are required.

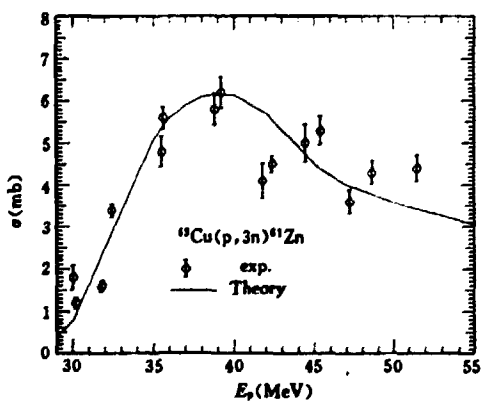

Fig. 1 The excitation function of ^{63}Cu(p,3n)^{61}Zn reaction

2 NUCLEAR REACTION THEORY AND MODEL CALCULATION

Many CPND needed for application are either very difficult to measure or have to wait for being measured for unpredictable time delays. To a large extent due to the practical requirements, nuclear reaction theories and models have been developed to the extent, that with appropriate parameters based on related available experimental data the required limited accuracies for some of those "unmeasurable" data can approximately be met. These developments concern particularly the theoretical description of fission process, improvement in the statistical and optical models of nuclear reaction, the introduction of pre-equilibrium and multistep processes in the description of nuclear reaction and a further understanding of the physical foundations of nuclear model parameters. Parallel to these theoretical developments powerful computer codes have been developed which allow very detailed calculations of nuclear reaction data for structural and fissionable materials.

The present power of appropriately parameterised nuclear reaction theories and nuclear model calculation can be described as follows :

(1) They can be employed for inter- and extra-polation of experimental results[5], see Fig. 2;

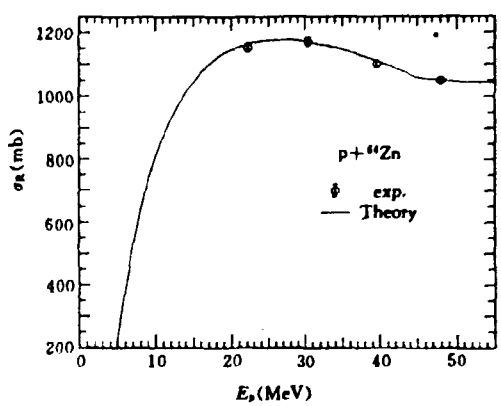

Fig. 2 The reaction cross sections of p+^{64}Zn
— CMUP2 calculation

(2) They can be used for the prediction of unknown nuclear data such as reaction cross section, angular and energy distributions as well as double differential cross section etc.[6], see Fig. 3;

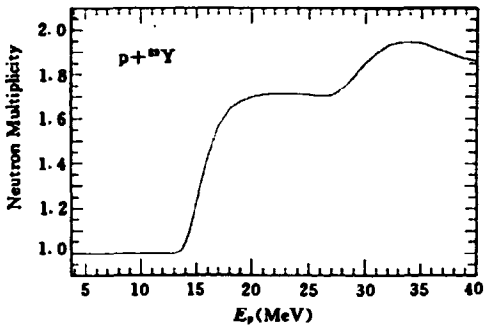

Fig. 3 The calculated neutron multiplicity of ^{89}Y induced by proton below 40 MeV

(3) They can be used to check the internal consistency between measurements of different nuclear data of the same nuclides or neighboring nuclides and can occasionally help in deciding among discrepant experimental results[7], as shown in Fig. 4;

The isomeric cross section ratios for reaction $^{55}Mn(\alpha,n)^{58}Co$ were determined by S. Iwata (1962)[8], T. Matuso (1965)[9] and Long Xianguan et al. (1989)[7]. The theoretical calculation was performed with Huizenga and Vandenbosch method[10], it trends towards the experimental data of S. Iwata[8] and Long Xianguan et al.[7]. The latter is a newer and more accurate measurement, because high resolution γ–spectrometry technique was used.

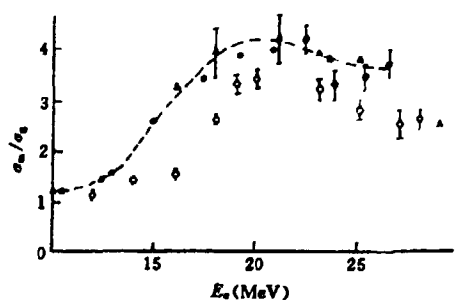

Fig. 4 Isomeric cross section ratios for $^{55}Mn(\alpha,n)^{58}Co$ reaction

— Theoretical calculation; ▲ Iwata (1963); ○ Matuso (1965); ● Long Xianguan et al. (1989).

(4) They can be used to calculate the cross sections of numerous charged particle nuclear reactions with medium and high incident energy.

Some general and united codes for CPND have been set up at CNDC. For instance, a comprehensive R–matrix analysis RCA code[11] based on the multichannel and multilevel R–matrix theory[12] is for light nuclei; model calculation codes CMUP2[13] based on the optical model and the unified treatment of exciton model and evaporation model is for medium and heavy weight nuclei and CFUP1[14] based on MUP2[15] code for fissile ones, they can be used to calculate the related CPND in the energy region from threshold to 50 MeV, and will to 100 MeV according to the plan of 1993. See Fig. 5[16].

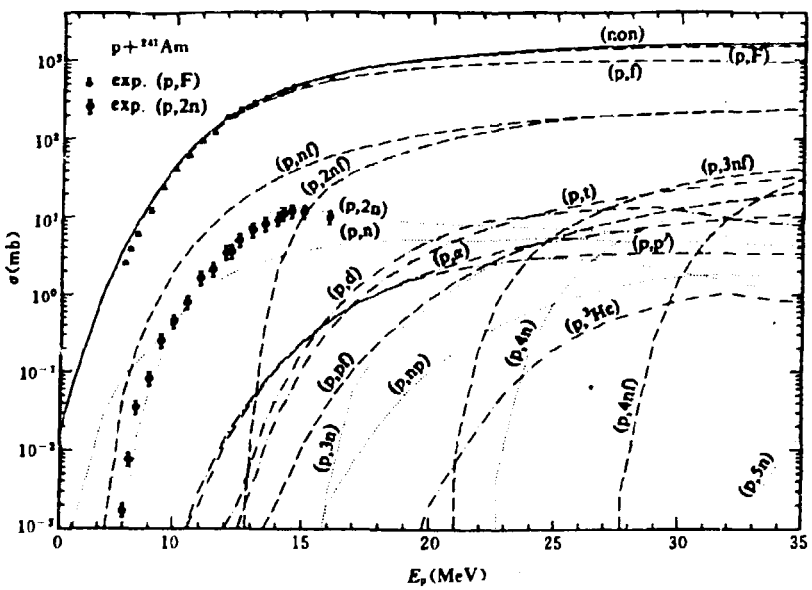

Fig. 5 The calculated particle emission cross sections in reaction p+^{241}Am below 35 MeV

— CFUPI calculation

3 SYSTEMATICS RESEARCH

The CPND of the nuclides which have a short life time or very low abundance are either scarce or scattered, some of these data can complemented by systematics.

The method settled a problem by from individuality to generality such as systematics has been applied in many sciences.

If systematical behavior can be found out from existing experimental data of other nuclei, unknown physical quantities can be derived from known ones with the aid of systematics research.

A series of systematics research on neutron data have been done at CNDC, such as average total radiative widths[17], thermal fission cross sections of actinides[18], (n,2n)[19], (n,charged–particle) and (n,γ) cross sections[20~23].

The systematicses of (p,n), (p,2n) and (d,n), (d,2n) reaction cross sections are being studied by means of simplified model formulas and empirical parameters at CNDC. The results will be published in "Communication of Nuclear Data Progress".

4 COMPREHENSIVE RECOMMENDATION

A final comprehensive recommendation is usually necessary after the evaluations for various channels accomplished individually, when a complete set of all the partial reaction data is required.

(1) Generally, the comprehensive recommendation is mainly based on the evaluated measured data, the model theory calculation and systematics results are usually used to make up the deficiencies of experimental data;

(2) A comprehnsive reevaluation must be done in the case that the individual evaluations do not meet the physical constraint condition, i. e. the nonelastic scattering cross section is not equal to the sum of all the partial cross sections.

In this case, some cross sections were reevaluated and adjusted firstly to make them to be self–consistent in the experimental errors. Then the reevaluated data of various reaction channels were fitted jointly to a self–consistent data set by measns of one of the following methods.

(1) To obtain the cross section of a specified reaction channel from other various channels according to certain physical relation. For example, a reaction cross section (usually they are deficient in measured data or with poor accuracy) can be deduced from the nonelastic scattering cross section minus the sum of all the other partial reaction cross sections;

(2) To make the excitation functions of various reaction channels self–consistent by the aid of simulteneously fitting of the various individual evaluations with the B–spline function or polynomial.

If there is a need for the data of a specific reaction channel but not for a complete set of all the partial reaction channels, the basic principles of comprehensive recommendation can be given as follows :

(1) There are more accurate and enough experimental data, the recom-

mended values are taken from evaluated ones;

(2) If experimental data are scarce, theoretical model calculation or systematics can represent them well, model or systematics calculation can be accepted, see Fig. 6[5].

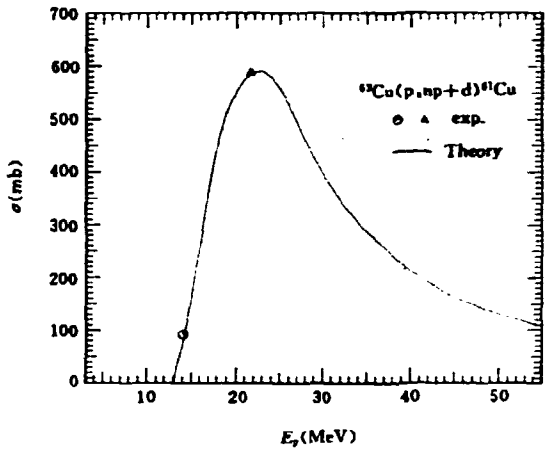

Fig. 6 The excitation function of $^{63}Cu(p,np+d)^{61}Cu$ reaction

5 SUMMARY

Using mentioned–above charged–particle evaluation techniques, CNDC has evaluated thermal nuclear reaction cross sections for fusion application and activation cross sections of intermediate and heavy nuclei for isotopes production and activation analysis, such as $^{2}H(d,n)^{3}He$, $^{2}H(d,p)^{3}H$, $^{3}H(d,n)^{4}He$, $^{3}He(d,p)^{4}He$, $d+^{6,7}Li$, $t+^{6,7}Li$, $^{3}He+^{6,7}Li$ and $^{56}Fe(p,\gamma)^{57}Co$, $^{57}Fe(p,n)^{57}Co$, $^{235}U(d,2n)^{235}Np$, $^{235}U(p,n)^{235}Np$. The evaluated results have satisfied the needs of the users.

However, the model calculation program for light nuclides still need to be set up at CNDC. The existing codes CMUP2 and CFUP1 will be developed in the energy region from threshold to 100 MeV or more. It is necessary for CNDC to make a further research on the systematics and covariance of CPND. A problem awaiting solution in the world is how to establish a set of standard data of monitor for CPND measurements.

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EVALUATION OF NEUTRON NUCLEAR DATA FOR ^{7}Li

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ABSTRACT

New complete neutron data for ^{7}Li have been evaluated for CENDL-2. It updates our work in 1978 for CENDL-1 to extend incident neutron energy range from 10^{-5} eV to 20 MeV. Combining new experimental data and benchmark testing, the tritium production cross section were improved. The comparison of present evaluation with ENDF/B-6 and JENDL-3 has been made.

INTRODUCTION

^{7}Li is an indispensable of breeding material from its potential use for fusion energy application. Therefore, the neutron nuclear data of ^{7}Li are important for improving fusion reactor design. After CENDL-1 was completed, lot of experimental data were carried out by many laboratories. For tritium production cross section, there exist large differences among the data from different laboratories measured before 1979. The recently measured ones are smaller in value, and differences occur only when $E_n > 8$ MeV. In fact, the benchmark testing results show that old ones are too large. An accuracy 3 % of the cross section is requested. The tritium production cross section of neutron interaction with ^{7}Li was evaluated in 1990[1].

The inelastic scattering to 4.63 MeV state accounts for bigger ratio of the total $^{7}Li(n,n't)\alpha$ reaction. There are large differences among measured values. At first, the accurate data were analysed and evaluated for the differential inelastic cross section to 4.63 MeV state. In order to calculate theoretically the data, the microscopic DWBA theory were used. The calculated inelastic scattering differential cross section can reproduce the experimental data very well. Now other cross sections and angular distributions as well as secondary energy neutron spectra are also recommended. Consequently, new complete neutron

data for ^{7}Li have been presented for CENDL-2 to reflect the new information for the experimental data.

1 DATA ANALYSIS AND EVALUATION

1.1 Total Cross Section

The total cross section was evaluated based on the measured data by Harvey[2], Goulding[3], Foster[4], Lamaze[5], and thermal energy data recommended by Mughabghab[6]. Therefore, in the energy range above 100 keV, there is no large change from CENDL-1. New experimental data were considered. Below 100 keV, the total cross section was the sum of thermal scattering cross section and the radiative capture cross section. The thermal scattering cross section is 0.97 b, which was recommended by Mughabghab[6].

The comparison of our recommended with others for the total cross section is shown in Fig. 1.

1.2 Elastic Scattering Cross Section

As mentioned above, the thermal scattering cross section of 0.97 b was adopted below 100 keV. Above 100 keV energy range, the elastic scattering cross sections were obtained by subtracting the nonelastic reaction cross section from total cross section. The results are consistent with new measured data by Chiba[7], Shen[8] within experimental error.

1.3 Radiative Capture Cross Section

Radiation capture of neutron by ^{7}Li leads to an unstable isotope ^{8}Li, which decays with about a 0.9 second half-life by emitting electrons with a maximum energy of 13 MeV. The residual nucleus, ^{8}Be, further decays into two alpha particles in about 10^{-15} second. Since the spin and parity of the ground state of ^{8}Li are 2 even, and the spin and parity of the ground state of ^{7}Li are 3/2 odd, the excited state of ^{8}Li formed by S-wave neutron capture in ^{7}Li will decay to the ground state by electric dipole emission. The neutron radiative capture cross section of ^{7}Li was measured by Imhof[9] in the neutron energy from 40 to 1000 keV. The cross section were measured relatively to the known cross sections of the $^{6}Li(n,t)\alpha$ and the $^{127}I(n,\gamma)^{128}I$ reactions. In the measurement, the difference of $^{7}Li(n,\gamma)$ cross section existed due to use the early normalization cross section of $^{6}Li(n,t)\alpha$ and $^{127}I(n,\gamma)^{128}I$ reactions. Now, the

cross section, especially in 700 to 1000 keV energy range , are more closed each other after using the new normalization cross sections from ENDF / B–6 in the present evaluation.

The thremal energy data were also adopted from the recommended data by Mughabghab[6]. Therefore, The cross section out of 40 to 1000 keV energy range are expressed as

$$\sigma_{n,\gamma} = 7.22 \times 10^{-3} [\ E_n(\ eV\ )\ ]^{-1/2}\ ,\ (\ b\ )$$

The evaluated result is shown in Fig. 2

1.4 (n,2n) and (n,d) Reaction Cross Sections

For these reaction cross sections, the experimental data could be found only at a few energy points. The (n,2n) reaction cross section were measured by McTaggart[10], Ashby[11], Mather[12] and Chiba[7]. According to the new measured data by Chiba, the evaluated (n,2n) cross sections in CENDL–1 were adjusted slightly. The evaluated result is shown in Fig. 3.

The angular distribution of neutron emitted from ^{7}Li(n,2n) reaction was adopted from experimental data[7].

The ^{7}Li(n,d) reaction data was very scarce, the evaluated ^{7}Li(n, d) reaction cross section were recommended referring to the JENDL–3 values.

1.5 Inelastic Scattering Cross Section

1) The first level to 0.478 MeV

In most experiments the inelastic scattering cross section to the first 0.478 MeV state cannot be separated from the elastic scattering cross section. But the ^{7}Li(n,n'γ) reaction cross sections were measured by Morgan[13], so the cross section to the first level 0.478 MeV cross section could be obtained from the measurement.

2) The second level (4.63 MeV)

In the ^{7}Li(n,n't)α reaction, the inelastic scattering cross section to 4.63 MeV state accounts for about half of the total tritium production cross section. However, large difference exists among the data collected from different laboratories measured before 1992. The experimental data for ^{7}Li(n,n't)α reaction to 4.63 MeV state were measured mainly by 18 laboratories[7, 14~30]. The existing data are mainly in 6 to 14 MeV energy range, because most of the

measurements were performed with a pulsed monoenergetic neutron source in which case the secondary energy can be measured by the time-of-flight (TOF) method.

After analyzing the collected data, to find reasons for these deviation, the possible effect for extraneous background are recognized. This evaluation is mainly based on the experimental data in which were used enriched ^{7}Li sample and TOF spectrometer with good time resolution and high effect-to-background ratio. The scarce data were calculated by using perturbation theory in form of a microscopic DWBA.

The evaluated experimental data and the calculated results were fitted with orthogonal polynomial method, so the evaluated data were obtained. It was shown in Fig. 4 with experimental data and other evaluations.

3) Tritium production cross section

The microscopic data for ^{7}Li(n,n't)α reactions were measured mainly by 18 laboratories[7, 15, 16, 19, 20, 26, 31~42], large discrepancy exists among the data measured before 1979. The recently measured ones are smaller in values, and discrepancy occurs only when $E_n > 8$ MeV. In fact, the benchmark testing results show that the old ones are too large[43~45]. We have investigated and analysed the method of the cross sections measurement. The key effects on the experimental accuracy are the sample purity, collection and extraction of the tritium after irradiation and the method of tritium determination. The adoption of the enriched 99.9 % ^{7}Li sample and some new techniques of keeping fresh target are important to reduce the effect of the neutrons with lower energies.

Only a few data measured by TOF are available because with this technique a large amount of measurements is needed. Still Lisowski[26] and Chiba[7] have measured neutron spectra at more than 10 angles for several incident neutron energies by using high resolution TOF spectrometers, the deduced tritium production cross section are rather accurate.

In the present evaluation all experimental data up 1992 were collected, compared and analysed. The data from[20, 26, 36~42] were adopted, and the recommended values are consistent with the benchmark testing results, as shown in Fig. 5 together with other evaluations.

2 RECOMMENDATION AND DISCUSSION

Our recommended data are compared with JENDL-3 and ENDF / B-6. The results are shown in Figs. 1~5 with experimental data. It was shown from these results that :

2.1 The evaluated tritium production cross section are well consistent with the experimental values. Our evaluated values are close to the recently measured data by JAERI and University of Tokyo[45] with new techniques and fusion neutron source facility, especially from 13 to 15 MeV very well. (see Fig. 5)

2.2 In the evaluated $^{7}Li(n,n't)\alpha$ reaction cross sections to 4.63 MeV state, the newer experimental data were adopted in which the possible effect for extraneous background were recognized. Our recommended values are consistent with JENDL–3, but ENDF / B–6 are systematic higher than ours. (see Fig. 4)

2.3 For the experimental data on $^{7}Li(n,\gamma)$ radiative capture cross section, the scatters of experimental data become very little due to we corrected the normalization cross sections by ENDF / B–6. Therefore, the recommended data are reliable from 40 to 1000 keV energy range. (see Fig. 2).

2.4 The DWBA were used to calculated the inelastic scattering cross section to the excited 0.478 MeV and 4.63 MeV states in our evaluation. Because it have not yet given the state functions for the states higher than 4.63 MeV, the results for 6.68 MeV state by Chiba[30] were adopted, which was based on coupled–channel calculation.

For other discrete level data of $^{7}Li(n,n't)\alpha$ reaction, JENDL–3 data were also adopted. For continuum state, it was obtained by subtracting the 4.63, 6.68 and 7.467 MeV state from tritium production cross section of ^{7}Li.

At present evaluation, the important data concerned n + ^{7}Li were evaluated and recommended and these evaluated results could reproduce the experiment data very well. During our evaluation, the evaluated data for ENDF / B–6 were reviewed, and the discussion was also done with Chiba[47] who is author of new measurement data and evaluation of revision of JENDL–3 for ^{7}Li.

Some scarce data measured were calculated by using R–matrix and Coupled– channel theory. Because the individuality of ^{7}Li is very strong, the calculated Code by Zhu Yaoyin[48] could give its results at some energy points. Therefore, in this case others scarce data measured such as the double–differential data were supplemented from JENDL–3 after they were checked and analysed. The recommended DDXs were calculated based on the experimental data from Osaka University at 14 MeV and Tohoku University at 6.0, 14.2 MeV using enrich sample (99.9 % in ^{7}Li). Their evaluated data could reproduce the secondary neutron energy spectra excellent.

The a few body theory is investigating by Liu Funjing[49] and the calculated code is improving by Zhu Yaoyin[48]. The part of scarce experimental data will calculated so as to revise our evaluation in the future.

3 CONCLUDING REMARK

The neutron nuclear data of ^{7}Li were revised for CENDL–2 by taking account of the experimental data after the CENDL–1 evaluation. Main emphasis was on the tritium production cross section and some discrepancy data among some evaluated data from several laboratories.

3.1 The evaluated tritium production cross section were consistent with the benchmark testing results. The measured data[50] with new techniques at fusion neutron source around 14 MeV were published after our evaluation[1]. The values are higher than the values of JENDL–PRT and over lower than ENDF / B–5, but in agreement with our evaluation[1]. At present, these evaluated results are consistent very well with the measured data around 14 MeV.

3.2 For 4.63 MeV state, there exists inconsistency among the measured cross section from 7 MeV to 14 MeV. According to the analysis of expérimental data, the values measured by Hogue[25] and Dekempenner[29] were systematic higher. Main reason was found, that the subtraction of the background neutron effects was not so good, and some were reasonable. The possible effect for extraneous background were from the subtraction of the background neutron, present the calculation of neutron inelastic (4.63 MeV level) scattering by ^{7}Li are low than the measured results by Hogue[25]. Our evaluated value are close to the new measured data by Chiba[30].

3.3 For radiative capture cross section, the measured data by Imhof[9] were corrected for normalization standard cross section in 40 to 1000 keV energy range. Therefore, our recommended data are more reliable.

ACNOWLEDGEMENT

The one of authors would like to thank Dr. S. Chiba for his helpful discussion on the evaluation at JAERI / NDC. They are also grateful to Drs. Zhu Yaoyin and Su Zongdi for their discussion in calculation problems, Drs. Liang Qichang, Liu Tong for using their treatment codes.

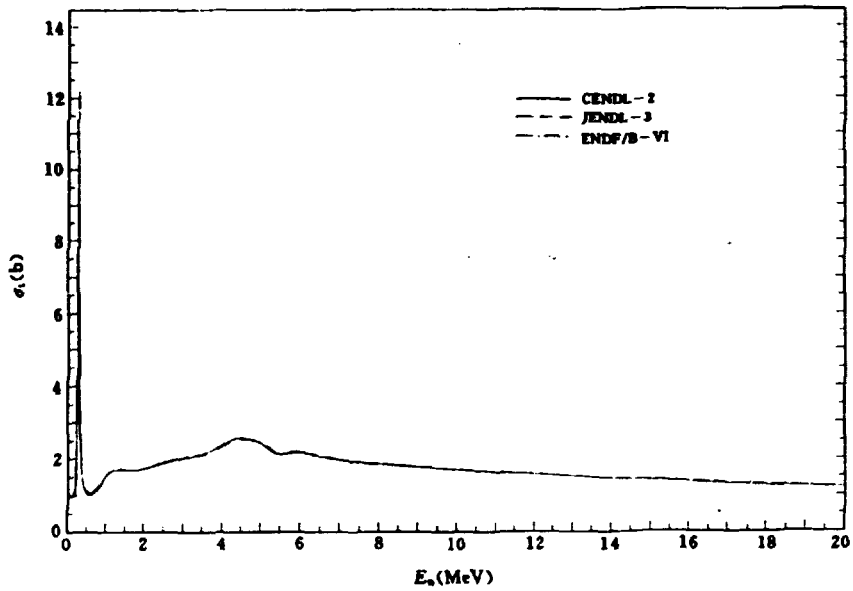

Fig. 1 The total cross section of ^{7}Li

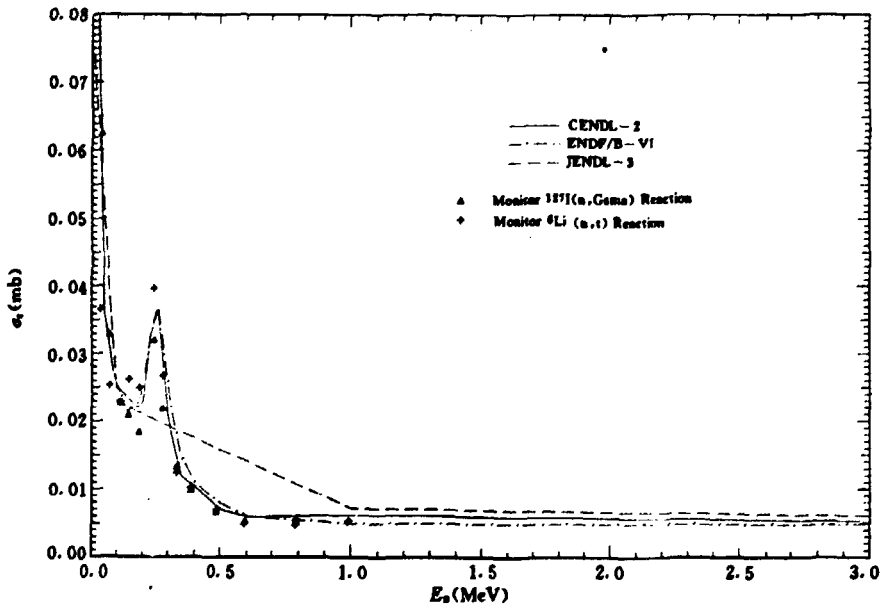

Fig. 2 The radiative capture cross section of ^{7}Li

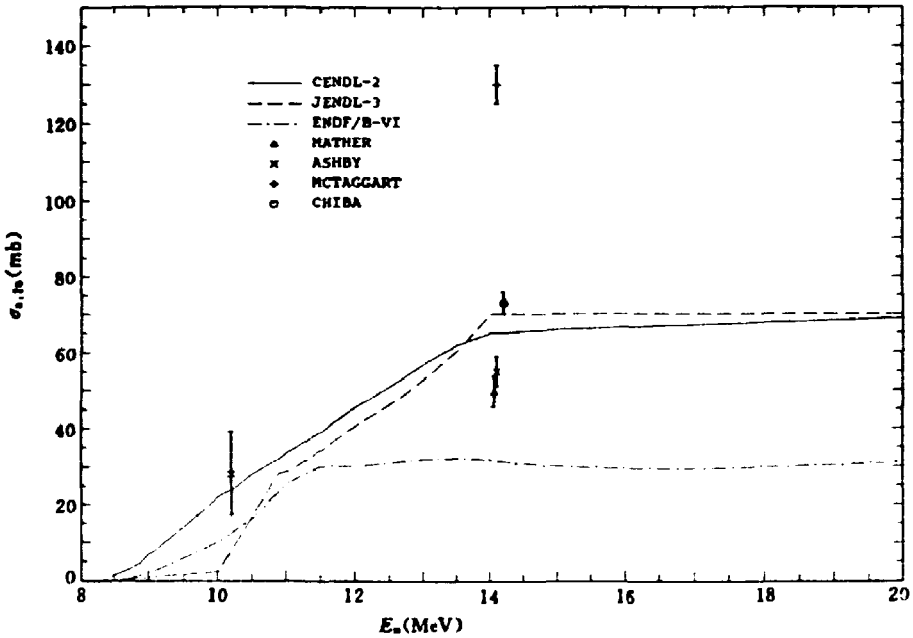

Fig. 3 The ^{7}Li reaction cross section

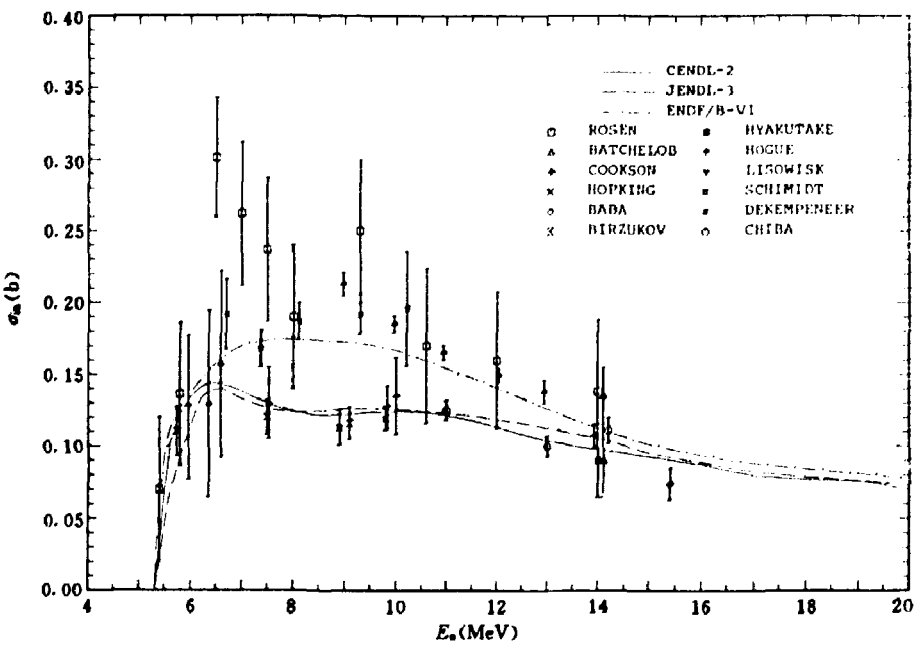

Fig. 4 The inelastic scattering cross section to 4.63 MeV state of ^{7}Li

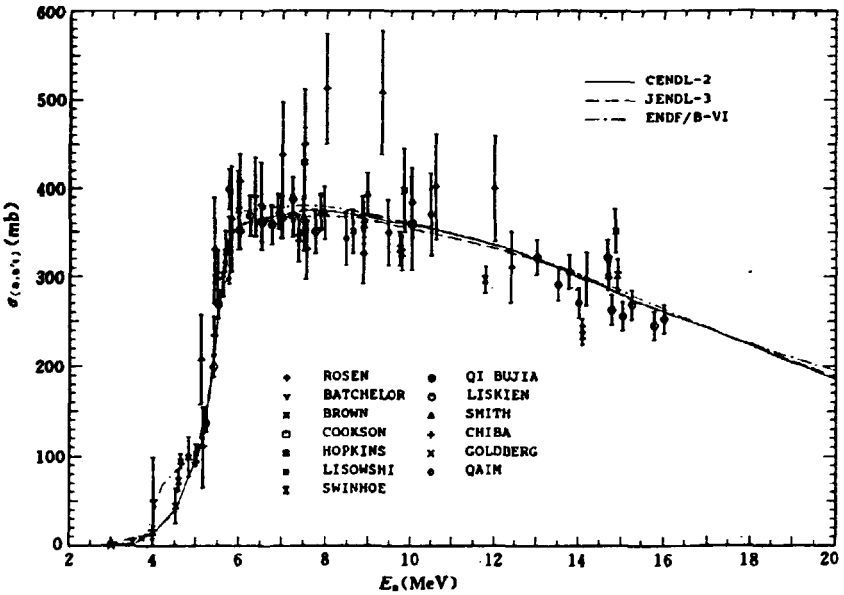

Fig. 5 The tritium production cross section of ^{7}Li

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REVISION ON RECOMMENDED DATA OF ^{238}U FOR CENDL-2

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For evaluation of neutron data of ^{238}U in 1991 version, we have revised as follows :

1 In neutron energy range from 50 to 500 keV, our recommended data of capture cross section in the 1991 version[1] was based on measured data collected by us before 1991. They are larger than expected ones from benchmark calculation.

Recently we have known that the NEACRP / NEANDC Working Group on International Evaluation Cooperation has intensively studied and resolved the problems of the capture cross section. It was convinced that the lower recommended data of capture cross section than average data of earlier measurements are reasonable[2]. From the 1991 Julich conference, we have obtained the new data measured by K. Kobayashi[3]. These data are in good agreement with the experimental data of L. E. Kazakov et al.[4].

Based on the data of K. Kobayashi et al. we have revised our evaluated data. Present revised data of capture cross section have been included in the new ^{238}U data of CENDL-2.

Revised data of capture cross section and their comparison with those of ENDF / B-6, JENDL-3 are shown in Figs. 1~3.

2 In the new version for recommended data of ^{238}U, the resonance parameters in the energy range below 50 keV are taken from JENDL-3 based on the demands of users and considering there are no discrepancy among the recommended data in the resonance energy range.

3 In the new version data of ^{238}U, other reaction cross sections are unchanged.

The new version data of ^{238}U have been collected in the CENDL–2. Results of benchmark calculation are in good agreement with the data[5].

ACKNOWLEDGEMENTS

Many thanks for Drs. Liu Tingjin and Liu Guisheng who gave us useful help during the revision.

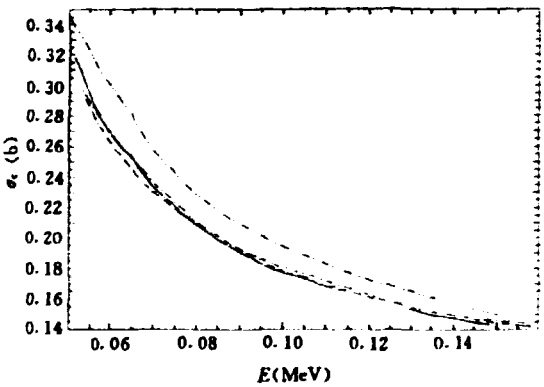
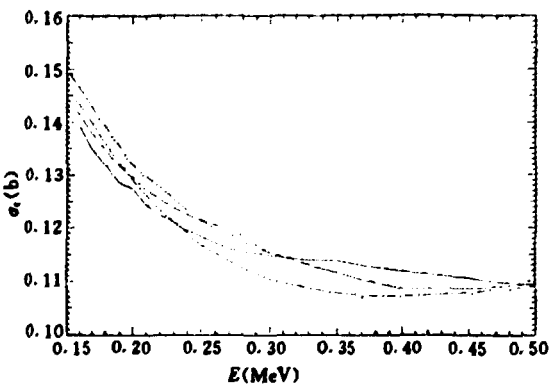
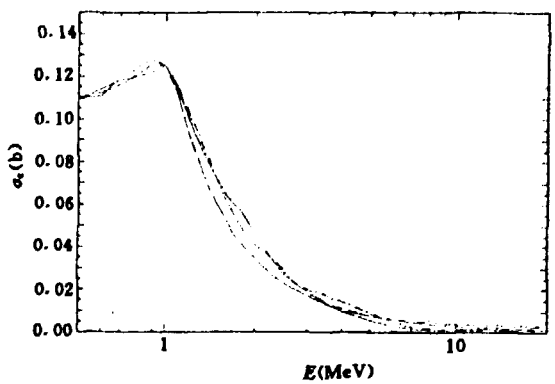


Fig. 1 Capture cross section of ^{238}U

—— ENDF / B–6; – – – JENDL–3; —·— CENDL–2; —·· — JEF–1.





Figs. 2 ~ 3 Capture cross section of ^{238}U

—— ENDF / B–6; – – – JENDL–3; —·— CENDL–2; —·· — JEF–1.

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PROGRESS ON THE EVALUATION OF CHARGED PARTICLE NUCLEAR REACTION DATA IN SICHUAN UNIVERSITY

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According to the assignment of the second meeting on CPND (Xian, 1989), the evaluations of excitation functions of 9 reactions induced by charged particles have been fulfilled. The evaluated nuclear reactions and the experimental works are listed in table 1.

Table 1 The evaluated nuclear reactions

Reaction	Related experimental work		Remark
	Energy Range (MeV)	References	
$^{56}Fe(p,2n)^{55}Co$	15.6~39	1) J. Inorg. & Nucl. Chem., 32, 1419(1970)	
	15.6~38.9	2) Intern. J. of Applied Radiation & Isotopes, 32, 25(1979)	Data of 2) are recommended
$^{55}Mn(\alpha,2n)^{57}Co$	12.9~38.4	1) J. Phys. Soc. Japan, 15, 545(1960)	
	13.2~38.5	2) J. Phys. Soc. Japan, 17, 1323(1962)	Results of 4 work are nearly consistent with each other, a curve through these points is recommended
	12.7~78.68	3) antwep, p. 599, (1982) EXFOR P0064	
	14.9~26.5	4) High Energy Physics & Nuclear Physics, 14, 444(1990)	
$^{94,96}Mo(d,x)$ $^{95m,96,97m}Tc$	2.4~12.7	1) J. Inorg. & Nucl. Chem., 38, 2289(1976)	Data given by 2) are recommended
	3.2~13.3	2) High Energy Physics & Nuclear Physics, 15, 827(1991)	
$^{48}Ti(p,\gamma)^{49}V$	13.3~44.7	1) J. Inorg. & Nucl. Chem., 40, 1845(1978)	In 5.1~12.6 MeV region data of 2) are recommended, but in 13.30~44.7 MeV data of 1) are recommended
	5.1~14.0	2) J. Phys. Soc. Japan, 14, 1269(1959)	
$^{55}Mn(p,np)^{54}Mn$	21.5	1) Phys. Rev., 99, 718(1955)	
	21.5~152.0	2) J. Phys. Radium., 22, 636(1961)	Data of 2) are recommended
Ni(p,x)^{52}Mn, ^{56,57}Co, ^{57}Ni	18.1~84.3	1) CSIR-FIS-89 EXFOR B0098	Data of 2) are recommended, but there are only two measurements for reaction Ni(p,x) Mn and divergence exists between 2) and 3), hence both of the data are given for being selected
	11.9~44.7	2) Z. Physik, A 286, 393(1978)	
	11.0~98.0	3) Atomnaja Energija, 62, 411(1987)	

Table 1 The evaluated nuclear reactions (continue)

Reaction	Related experimental work		Remark
	Energy Range (MeV)	References	
$^{52,53}Cr(p,2n)^{51,52}Mn$	21.5 370 400 22	1) Phys. Rev., 99, 718(1955) 2) Phys. Rev., 138, 2069(1963) 3) J. Inorg. & Nucl. Chem., 31, 1959(1969) 4) Atomnaja Energija, 39, 264(1984)	4 measurements in all, each of them had only done for one energy point
$^{50}Cr(d,n)^{51}Mn$	2～12	1) Nucl. Phys., 79 203(1966)	Data of 1) are recommended
$^{54,57}Fe(d,n)^{55,58}Co$	5～40 4.7～13.6 6.4～15.7	1) Phys. Rev., 179, 1104(1969) 2) Atomnaja Energija, 2, 169(1957) 3) Chinese J. Nucl. Tech., 4, 506(1984)	Data of 3) are recommended

PROGRESS ON NUCLEAR STRUCTURE AND DECAY DATA EVALUATION FOR A–CHAIN IN CHINA

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The nuclear structure and decay data (NSDD) are important data for the basic research of nuclear physics, applied research of nuclear techniques and engineering design of nuclear energy. The evaluations and updates of NSDD for $A = 1 \sim 266$ have been done respectively by members of the International Nuclear Structure and Decay Data Network. China Institute of Atomic Energy, Beijing, as Chinese responsible institution, has primary responsibility for evaluating and updating NSDD for $A = 51 \sim 56$ and $195 \sim 198$, and temporary for evaluating NSDD for $A = 61$, 170 and 172. The other members of Chinese NSDD evaluation group are from Department of Physics, Jilin University, Changchun, and Institute of Nuclear Research, Shanghai. The status of NSDD evaluation in China is summarized. The following has been put into Evaluated Nuclear Structure Data File in 1992,

$A = 61$ Nuclear Data Sheets, Vol. 67, 271 (1992)

$A = 196$ Nuclear Data Sheets (to be published in 1993)

updated,

$A = 56$ Nuclear Data Sheets, Vol. 67, 523 (1993)

$A = 54$ Nuclear Data Sheets (to be published in 1993)

NUCLEAR DATA SHEETS UPDATE FOR $A = 61$

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(CHINESE NUCLEAR DATA CENTER, IAE)

The 1983 version of the Nuclear Data Sheets for $A = 61$ was evaluated by L. P. Ekstrom et al.[1]. The Nuclear Data Sheets Update for $A = 61$ has been done on the basis of the nuclear reaction and nuclear decay experiments leading to all the nuclei with mass number $A = 61$ since cutoff date of last evaluation, October 1982. The most of evaluated data have been updated , or revised. The nuclei of updated data mainly are ^{61}Fe, ^{61}Co, ^{61}Ni, ^{61}Cu, ^{61}Zn and ^{61}Ga. The level properties and their γ radiations from reaction and decay experiments are presented by means of schemes or tables. The adopted levels and adopted γ radiations are shown in tables. The experimental methods, references and necessary comments are given in the text.

The updated version of Nuclear Data Sheets for $A = 61$ have been put into Evaluated Nuclear Structure Data File, Brookhaven National Laboratory, USA, and published[2].

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A NEW SET OF AVERAGE LEVEL SPACINGS FOR S-WAVE RESONANCE

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Zhao Zhixiang Zhou Delin

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In general,average level spacing is obtained from the analysing a set of resolved resonance parameters. A problem in the estimation of average level spacing is that usually many weak levels, which have small neutron width, are missed because of finite resolution and sensitivity in neutron experiments. Most of methods to correct level missing are only based on a cut-tailed Porter-Thomas distribution of reduced neutron widths, and the information in level position have not been used. The Bayesian approach developed by the authors[1,2] make it possible to simultaneously use the information in both neutron width and level position, therefore the estimate of $<D>$ is improved.

In this work, the Bayesian approach is used to evaluate s-wave average level spacings for about 210 target nuclei. The resolved resonance parameters to be analysed are taken from evaluated data of ENDF / B-6[3]. The prior estimates for the number of s-wave resonance, N_0, are calculated by using AVRPES code[4], which is developed on the basis of a cut-tailed Porter-Thomas distribution.

The Bayesian estimates for $<D_0>$ calculated in this work are given in table 1 with those given by Mughabghab[5], Reffo[6] and Ignatyuk[7]. In the table, N, means the number of resolved s-wave resonances and all of estimates for $<D_0>$ are in keV. It can be seen from the table that for some target nuclei there are large discrepancies among this work and others. One of the reasons for this discrepancy may come from that the resolved resonance parameter samples to be analysed for these targets are not perfect.

Table 1 Bayesian estimates of s-wave average level spacing

Target	N_s	This Work	BNL-325	Reffo	Ignatyuk
^{23}Na	4	7.460+1 ± 1.52+1		1.429+2 ± 3.61+1	
^{40}Ar	6	5.800+1 ± 1.20+1		7.532+1 ± 2.22+1	8.700+1 ± 1.30+1
^{45}Sc	78	1.280+0 ± 8.00-2	1.300+0 ± 1.00-1	1.450+0 ± 1.50-1	1.300+0 ± 1.00-1
^{50}Cr	64	1.210+1 ± 8.00-1	1.500+1 ± 2.00+0	1.346+1 ± 3.54+0	1.500+1 ± 2.00+0
^{52}Cr	23	4.000+1 ± 4.00+0	4.200+1 ± 5.00+0		4.500+1 ± 6.00+0
^{53}Cr	29	6.330+0 ± 6.20-1	7.100+0 ± 1.20+0	6.550+0 ± 1.75+0	7.100+0 ± 1.00+0
^{54}Cr	14	3.700+1 ± 4.00+0	2.600+1 ± 7.00+0	3.194+1 ± 6.39+0	6.000+1 ± 9.00+0
^{55}Mn	50	2.170+0 ± 1.70-1	2.700+0 ± 4.00-1	2.700+0 ± 4.00-1	2.700+0 ± 4.00-1
^{54}Fe	61	1.440+1 ± 1.00+0	1.300+1 ± 2.00+0		2.040+1 ± 2.70+0
^{56}Fe	36	2.300+1 ± 2.00+0	1.700+1 ± 2.00+0		2.500+1 ± 5.00+0
^{57}Fe	22	6.650+0 ± 6.80-1	6.000+0 ± 1.00+0		6.500+0 ± 1.00+0
^{58}Fe	13	3.350+1 ± 4.70+0	3.500+1 ± 1.50+1		3.500+1 ± 1.50+1
^{59}Co	100	9.700-1 ± 5.00-2	1.100+0 ± 1.00-1	1.340+0 ± 3.40-1	1.100+0 ± 1.00-1
^{58}Ni	62	1.290+1 ± 9.00-1	1.370+1 ± 2.00+0	1.533+1 ± 2.65+0	1.670+1 ± 2.10+0
^{60}Ni	30	1.390+1 ± 1.30+0	1.600+1 ± 2.50+0	1.494+1 ± 2.03+0	1.600+1 ± 2.50+0
^{61}Ni	31	1.860+0 ± 1.80-1	1.800+0 ± 3.00-1	2.135+0 ± 3.61-1	1.800+0 ± 3.00-1
^{62}Ni	29	1.700+1 ± 1.60+0	1.910+1 ± 3.60+0	1.825+1 ± 4.00+0	1.910+1 ± 3.60+0
^{64}Ni	28	1.870+1 ± 1.90+0	1.990+1 ± 3.60+0	1.980+1 ± 8.63+0	1.990+1 ± 3.60+0
^{63}Cu	184	5.040-1 ± 2.00-2	3.200-1 ± 3.00-2	1.452+0 ± 3.29-1	1.040+0 ± 1.10-1
^{65}Cu	129	7.370-1 ± 3.50-2	5.100-1 ± 6.00-2	1.148+0 ± 3.19-1	1.470+0 ± 1.90-1
^{72}Ge	6	7.320-1 ± 1.44-1	9.600-1 ± 4.00-1	3.500+0 ± 8.00-1	9.600-1 ± 4.00-1
^{73}Ge	10	4.000-2 ± 7.00-3	8.200-2 ± 2.00-2	1.650-1 ± 2.00-2	8.200-2 ± 2.00-2
^{74}Ge	3	6.430-1 ± 1.93-1	3.000+0 ± 1.50+0	5.000+0 ± 3.00+0	3.000+0 ± 1.50+0
^{75}As	32	6.900-2 ± 7.00-3	7.500-2 ± 5.00-3		7.500-2 ± 5.00-3
^{74}Se	7	3.200-1 ± 6.50-2	4.200-1 ± 2.40-1	8.000-1 ± 1.00-1	4.200-1 ± 2.00-2
^{76}Se	11	6.140-1 ± 9.90-2	6.670-1 ± 2.70-1	8.000-1 ± 2.00-1	6.670-1 ± 2.70-1
^{77}Se	22	1.090-1 ± 1.20-2	1.460-1 ± 3.00-2	1.460-1 ± 3.00-2	1.460-1 ± 3.00-2
^{78}Se	6	1.090+0 ± 1.90-1	1.390+0 ± 5.00-1	2.400+0 ± 4.00-1	1.390+0 ± 5.00-1
^{80}Se	5	1.120+0 ± 2.70-1	3.500+0 ± 1.50+0	3.000+0 ± 4.00-1	3.500+0 ± 1.50+0
^{79}Br	13	2.800-2 ± 4.00-3	4.700-2 ± 5.00-3	5.500-2 ± 8.00-3	4.700-2 ± 5.00-3
^{81}Br	5	3.800-2 ± 9.00-3	9.400-2 ± 1.50-2	1.720-1 ± 2.50-2	9.400-2 ± 1.50-2
^{78}Kr	3	2.130-1 ± 6.70-2	2.300-1 ± 6.00-2		2.300-1 ± 6.00-2
^{80}Kr	4	1.690-1 ± 4.00-2	2.000-1 ± 6.00-2		2.000-1 ± 6.00-2
^{83}Kr	2	7.700-2 ± 2.40-2	3.260-1 ± 2.00-1		3.260-1 ± 2.00-1
^{84}Kr	3	3.990-1 ± 1.08-1	2.420-1 ± 1.30-1		2.420-1 ± 1.30-1

Target	N_s	This Work	BNL-325	Reffo	Ignatyuk
^{85}Rb	75	2.140-1 ± 1.30-2	2.000-1 ± 4.50-2	2.200-1 ± 2.00-2	2.000-1 ± 4.50-2
^{87}Rb	14	1.460+0 ± 2.00-1	2.640+0 ± 8.80-1	2.400+0 ± 6.00-1	2.640+0 ± 8.80-1
^{84}Sr	9	3.290-1 ± 5.60-2	3.830-1 ± 1.30-1	4.160-1 ± 1.50-1	3.830-1 ± 1.30-1
^{86}Sr	7	1.800+0 ± 3.00-1	5.000-1 ± 6.60-2		3.000+0 ± 1.00+0
^{87}Sr	10	1.900-1 ± 2.70-2	1.210-1 ± 1.30-2	9.600-1 ± 3.00-1	1.210-1 ± 1.30-2
^{88}Sr	4	2.700+1 ± 6.00+0	2.500+1 ± 5.00+0	5.500+1 ± 5.00+0	4.000+1 ± 1.00+1
^{89}Y	34	2.800+0 ± 2.00-1	4.000+0 ± 4.00-1	4.400+0 ± 1.00+0	4.000+0 ± 4.00-1
^{90}Zr	21	7.800+0 ± 7.00-1	6.400+0 ± 1.10+0	1.050+1 ± 2.50+0	8.600+0 ± 1.60+0
^{91}Zr	35	6.140-1 ± 4.80-2	5.700-1 ± 1.00-1	8.200-1 ± 8.00-2	6.400-1 ± 1.20-1
^{92}Zr	15	6.340+0 ± 8.60-1	2.600+0 ± 7.00-1	6.000+0 ± 8.00-1	3.100+0 ± 1.00+0
^{94}Zr	22	3.400+0 ± 4.00-1	3.600+0 ± 8.00-1	3.800+0 ± 7.00-1	3.800+0 ± 1.00+0
^{96}Zr	8	9.500+0 ± 1.60+0	1.300+1 ± 4.00+0	1.530+1 ± 3.90+0	1.300+1 ± 4.00+0
^{93}Nb	147	4.500-2 ± 2.00-3	4.400-2 ± 4.00-3	1.050-1 ± 1.00-2	9.000-2 ± 2.00-2
^{94}Nb	2	3.080-2 ± 1.54-2			
^{92}Mo	8	1.630+0 ± 2.70-1	2.100+0 ± 3.00-1	3.000+0 ± 3.00-1	3.600+0 ± 7.00-1
^{94}Mo	5	7.490-1 ± 1.81-1	9.750-1 ± 2.60-1	2.265+0 ± 5.00-1	1.150+0 ± 3.50-1
^{95}Mo	25	7.500-2 ± 8.00-3	5.500-2 ± 8.00-3	1.150-1 ± 4.50-2	9.100-2 ± 1.10-2
^{96}Mo	4	7.470-1 ± 1.91-1	8.500-1 ± 4.50-2		9.500-1 ± 2.80-1
^{97}Mo	30	4.300-2 ± 4.00-3	3.200-2 ± 3.00-3	6.000-2 ± 1.50-2	4.200-2 ± 1.50-2
^{98}Mo	5	7.030-1 ± 1.61-1	9.700-1 ± 2.00-1		9.700-1 ± 2.00-1
^{100}Mo	3	8.660-1 ± 2.72-1	4.000-1	6.500-1 ± 1.00-1	7.000-1 ± 5.00-2
^{99}Tc	42	1.610-2 ± 1.30-3	1.070-2 ± 1.80-3		1.760-2 ± 1.00-3
^{99}Ru	5	1.450-2 ± 3.00-3	2.500-2 ± 2.00-3	2.600-2 ± 5.00-3	2.500-2 ± 2.00-3
^{101}Ru	7	1.340-2 ± 2.50-3	1.600-2 ± 2.00-3	9.400-2 ± 2.00-2	1.800-2 ± 2.00-3
^{104}Ru	4	2.640-1 ± 7.20-2	1.400-1 ± 1.70-2		3.000-1 ± 7.50-2
^{103}Rh	59	2.440-2 ± 1.70-3	1.600-2 ± 1.00-3		3.100-2 ± 3.00-3
^{105}Pd	80	1.020-2 ± 5.00-4	1.000-2 ± 5.00-4	1.300-2 ± 3.00-3	1.030-2 ± 7.00-4
^{107}Pd	65	1.200-2 ± 7.00-4	1.500-2 ± 3.00-3	1.600-2 ± 3.00-3	1.140-2 ± 9.00-4
^{107}Ag	73	2.720-2 ± 1.50-3	1.600-2 ± 3.00-3	4.300-2 ± 5.00-3	2.200-2 ± 2.00-3
^{109}Ag	83	2.690-2 ± 1.50-3	1.400-2 ± 2.00-3	3.000-2 ± 5.00-3	1.870-2 ± 1.30-3
^{110}Cd	40	1.760-1 ± 1.50-2	1.550-1 ± 2.00-2	1.700-1 ± 2.50-2	1.550-1 ± 2.00-2
^{111}Cd	63	2.800-2 ± 2.00-3	2.000-2 ± 4.00-3	3.300-2 ± 2.00-3	2.000-2 ± 4.00-3
^{112}Cd	31	1.580-1 ± 1.50-2	1.900-1 ± 2.50-2	1.450-1 ± 2.00-2	1.900-1 ± 2.50-2
^{113}Cd	12	2.050-2 ± 3.00-3	2.100-2 ± 4.00-3	4.000-2 ± 3.00-3	2.100-2 ± 4.00-3
^{114}Cd	22	1.510-1 ± 1.80-2	2.350-1 ± 3.50-2	2.980-1 ± 6.30-2	2.350-1 ± 3.50-2

Target	N_s	This Work	BNL-325	Reffo	Ignatyuk
^{116}Cd	7	3.790-1 ± 7.80-2	3.900-1 ± 9.00-2	5.900-1 ± 1.00-1	3.900-1 ± 9.00-2
^{113}In	9	4.600-3 ± 8.00-4	9.000-3 ± 2.00-3	2.600-2 ± 1.00-3	9.000-3 ± 2.00-3
^{115}In	89	1.100-2 ± 6.00-4	9.400-3 ± 2.00-4	9.300-3 ± 5.00-4	9.400-3 ± 9.00-4
^{112}Sn	5	1.500-1 ± 2.90-2	1.550-1	1.540-1 ± 3.00-2	1.570-1 ± 5.20-2
^{114}Sn	4	2.620-1 ± 6.40-2		2.800-1 ± 4.00-2	2.830-1 ± 1.06-1
^{115}Sn	3	3.700-2 ± 9.00-3		1.000-1 ± 2.00-2	5.000-2
^{116}Sn	4	2.780-1 ± 6.20-2		5.000-1 ± 5.00-2	6.290-1 ± 9.80-2
^{117}Sn	10	5.100-2 ± 9.00-3	4.800-2 ± 6.00-3		5.500-2 ± 5.00-3
^{118}Sn	3	4.070-1 ± 1.28-1	8.700-1 ± 3.90-1	4.800-1 ± 1.00-1	4.780-1 ± 1.48-1
^{119}Sn	3	7.300-2 ± 1.90-2	9.000-2 ± 2.00-2	1.100-1 ± 3.00-2	9.000-2 ± 2.00-2
^{120}Sn	7	1.358+0 ± 2.49-1	1.400+0 ± 1.70-1	3.400+0 ± 3.00-1	1.640+0 ± 2.00-1
^{122}Sn	3	8.200-1 ± 1.80-1			
^{124}Sn	2	1.103+0 ± 3.48-1			
^{121}Sb	60	1.410-2 ± 1.00-3	1.800-2 ± 2.00-3	1.850-2 ± 2.50-3	1.800-2 ± 2.00-3
^{123}Sb	48	2.690-2 ± 2.00-3	3.800-2 ± 4.00-3	4.200-2 ± 4.00-3	3.800-2 ± 4.00-3
^{122}Te	22	1.380-1 ± 1.50-2	1.320-1 ± 1.50-2	2.000-1 ± 5.00-2	1.320-1 ± 1.50-2
^{123}Te	26	2.320-2 ± 2.50-3	2.500-2 ± 4.00-3	2.900-2 ± 2.00-3	2.500-2 ± 4.00-3
^{124}Te	26	1.810-1 ± 1.80-2	1.300-1 ± 1.50-2	2.600-1 ± 5.00-2	1.470-1 ± 1.20-2
^{125}Te	30	3.700-2 ± 1.00-3	3.800-2 ± 3.00-3	5.625-2 ± 7.00-3	4.800-2 ± 4.00-3
^{126}Te	9	4.850-1 ± 7.70-2	2.100-1 ± 2.00-2	3.500-1 ± 2.00-2	4.700-1 ± 1.14-1
^{128}Te	4	6.230-1 ± 1.69-1	2.600-1 ± 3.00-2	6.880-1 ± 1.00-1	9.920-1 ± 3.50-1
^{130}Te	4	2.780+0 ± 5.30-1	8.700-1 ± 1.40-1	1.500+0 ± 3.00-1	8.700-1 ± 1.40-1
^{127}I	60	1.570-2 ± 1.10-3	9.700-3 ± 8.00-4	1.500-2 ± 5.00-3	1.450-2 ± 9.00-4
^{129}I	5	2.700-2 ± 6.00-3			
^{128}Xe	5	3.050-1 ± 5.00-2		4.000-1 ± 1.00-1	
^{129}Xe	69	5.700-2 ± 4.00-3	4.500-2 ± 6.00-3		3.200-2 ± 3.00-3
^{130}Xe	11	2.670-1 ± 4.00-2	1.900-1 ± 6.00-2	2.000-1 ± 2.00-2	1.900-1 ± 6.00-2
^{131}Xe	39	9.100-2 ± 8.00-3	7.000-2 ± 2.00-2	9.100-2 ± 2.10-2	7.400-2 ± 1.90-2
^{132}Xe	3	7.170-1 ± 1.55-1			
^{134}Xe	2	1.000+0 ± 5.00-1			
^{133}Cs	123	1.990-2 ± 1.00-3	2.065-2 ± 2.30-3	2.300-2 ± 2.50-3	2.270-2 ± 2.90-3
^{134}Cs	6	1.740-2 ± 3.00-3			2.700-2 ± 7.50-3
^{136}Cs	7	3.600-2 ± 7.00-3			
^{134}Ba	8	2.140-1 ± 4.00-2	1.270-1 ± 1.00-2		2.300-1 ± 6.00-2
^{135}Ba	28	3.800-2 ± 3.00-3	4.000-2 ± 7.00-3		4.000-2 ± 6.00-3

Target	N_s	This Work	BNL-325	Reffo	Ignatyuk
^{136}Ba	3	3.820-1 ± 1.01-1	4.300-1 ± 3.50-2		9.200-1 ± 2.00-2
^{137}Ba	8	1.480-1 ± 2.40-2	2.900-1 ± 4.00-2		3.800-1 ± 7.00-2
^{139}La	32	2.460-1 ± 2.20-2	2.080-1 ± 1.00-2		2.830-1 ± 5.00-2
^{141}Pr	15	8.000-2 ± 1.40-2	8.800-2 ± 9.00-3	1.550-1 ± 3.00-2	1.020-1 ± 2.00-2
^{142}Nd	5	8.500-1 ± 2.07-1	4.400-1 ± 5.20-2		6.630-1 ± 7.00-2
^{143}Nd	17	2.400-2 ± 3.00-3	4.500-2 ± 4.00-3	4.000-2 ± 4.00-3	3.650-2 ± 4.00-3
^{144}Nd	19	4.610-1 ± 5.60-2	4.300-1 ± 6.50-2	4.660-1 ± 7.80-2	4.320-1 ± 7.00-2
^{145}Nd	79	1.750-2 ± 1.10-3	2.200-2 ± 2.00-3	2.000-2 ± 2.00-3	1.700-2 ± 1.60-3
^{146}Nd	18	2.040-1 ± 2.60-2	2.350-1 ± 2.90-2	3.820-1 ± 8.00-2	2.900-1 ± 8.00-2
^{147}Nd	7	3.700-3 ± 7.00-4	5.000-3 ± 2.00-3		5.000-3
^{148}Nd	11	7.100-2 ± 1.20-2	1.400-1 ± 1.50-2	1.600-1 ± 1.00-2	1.670-1 ± 2.10-2
^{150}Nd	15	1.190-1 ± 1.70-2	1.740-1 ± 2.00-2	1.660-1 ± 1.10-2	1.640-1 ± 1.70-2
^{147}Pm	38	8.000-3 ± 7.00-4	3.600-3 ± 5.00-4		3.700-3 ± 1.40-4
^{147}Sm	140	5.800-3 ± 2.00-4	5.700-3 ± 5.00-4	6.785-3 ± 7.55-4	4.700-3 ± 1.20-3
^{149}Sm	29	3.100-3 ± 3.00-4	2.200-3 ± 2.00-4	2.450-3 ± 4.50-4	1.900-3 ± 3.00-4
^{150}Sm	11	4.600-2 ± 7.00-3	5.500-2 ± 9.00-3		4.900-2 ± 1.00-2
^{151}Sm	120	1.100-3 ± 1.00-4	1.200-3 ± 2.00-4	1.400-3 ± 4.00-4	1.000-3 ± 1.00-4
^{152}Sm	57	4.970-2 ± 3.50-3	5.180-2 ± 3.30-3	4.645-2 ± 7.05-3	4.600-2 ± 7.00-3
^{154}Sm	18	1.120-1 ± 1.40-2	1.150-1 ± 1.20-2	1.250-1 ± 2.00-2	1.110-1 ± 1.20-2
^{151}Eu	91	7.500-4 ± 4.00-5	7.300-4 ± 7.00-5	8.700-4 ± 2.10-4	7.000-4 ± 9.00-5
^{152}Eu	83	4.200-4 ± 2.00-5	2.500-4 ± 4.00-5		2.500-4 ± 4.00-5
^{153}Eu	71	1.250-3 ± 8.00-5	1.300-3 ± 2.00-4	1.240-3 ± 2.60-4	1.100-3 ± 2.00-4
^{154}Eu	59	9.300-4 ± 6.00-5	9.200-4 ± 1.70-4	9.000-3 ± 1.20-4	9.200-4 ± 1.70-4
^{155}Eu	7	4.300-3 ± 8.00-4		6.450-3 ± 1.65-3	4.800-3 ± 4.00-4
^{152}Gd	17	1.130-2 ± 1.40-3	1.500-2 ± 2.00-3	1.400-2 ± 3.20-3	1.500-2 ± 2.00-3
^{154}Gd	48	1.650-2 ± 1.20-3	1.450-2 ± 1.50-3		1.450-2 ± 1.50-3
^{155}Gd	92	1.770-3 ± 1.00-4	1.800-3 ± 2.00-4	1.700-3 ± 3.00-4	1.800-3 ± 3.00-4
^{156}Gd	30	4.400-2 ± 4.00-3	3.780-2 ± 5.50-3		3.800-2 ± 5.00-3
^{157}Gd	56	5.100-3 ± 4.00-4	4.900-3 ± 4.00-4	5.550-3 ± 1.05-3	4.900-3 ± 4.00-4
^{158}Gd	93	9.000-2 ± 5.00-3	8.500-2 ± 3.00-3		8.500-2 ± 1.00-2
^{160}Gd	44	2.180-1 ± 1.80-2	2.020-1 ± 2.00-2		2.020-1 ± 2.00-2
^{159}Tb	23	3.640-3 ± 3.90-4	3.900-3 ± 4.00-4	4.230-3 ± 7.35-4	4.400-3 ± 4.00-4
^{160}Dy	3	6.800-3 ± 2.20-3	2.730-2 ± 1.70-3	3.100-2 ± 4.00-3	2.730-2 ± 1.70-3
^{161}Dy	26	2.100-3 ± 2.00-4	2.670-3 ± 1.30-4	2.950-3 ± 2.80-4	2.670-3 ± 1.30-4
^{162}Dy	8	5.100-2 ± 1.00-2	6.460-2 ± 1.90-3	8.200-2 ± 1.74-2	6.460-2 ± 1.90-3

Target	N_s	This Work	BNL-325	Reffo	Ignatyuk
^{163}Dy	59	7.930-3 ± 5.60-4	6.850-3 ± 5.40-4	7.710-3 ± 8.60-4	6.800-3 ± 6.00-4
^{165}Ho	29	4.800-3 ± 5.00-4	4.600-3 ± 5.00-4	4.570-3 ± 5.60-4	4.600-3 ± 5.00-4
^{166}Er	50	3.800-2 ± 3.00-3	3.800-2 ± 3.00-3	4.650-2 ± 8.60-3	3.800-2 ± 2.00-3
^{167}Er	113	4.500-3 ± 2.00-4	4.000-3 ± 2.00-4	4.600-3 ± 6.00-4	4.650-3 ± 2.20-4
^{175}Lu	16	2.800-3 ± 3.00-4	3.450-3 ± 1.50-4		3.600-3 ± 3.00-4
^{176}Lu	21	1.800-3 ± 2.00-4	1.740-3 ± 1.70-4	2.300-3 ± 6.00-4	1.700-3 ± 2.00-4
^{174}Hf	10	1.850-2 ± 2.90-3	2.100-2 ± 5.00-3	1.610-2 ± 4.90-3	2.100-2 ± 5.00-3
^{176}Hf	22	3.400-2 ± 3.00-3	3.200-2 ± 7.00-3	4.900-2 ± 1.80-2	3.200-2 ± 7.00-3
^{177}Hf	99	2.500-3 ± 1.00-4	2.400-3 ± 3.00-4	2.900-3 ± 5.00-4	2.400-3 ± 3.00-4
^{178}Hf	25	6.700-2 ± 7.00-3	6.200-2 ± 1.10-2	2.230-1 ± 1.50-2	6.200-2 ± 1.10-2
^{179}Hf	49	4.600-3 ± 3.00-4	4.400-3 ± 2.00-4	1.250-2 ± 2.00-3	4.400-3 ± 2.00-4
^{180}Hf	29	1.830-1 ± 1.40-2	9.400-2 ± 1.10-2	2.450-1 ± 3.30-2	9.400-2 ± 1.10-2
^{181}Ta	75	3.960-3 ± 2.40-4	4.170-3 ± 4.00-5	4.000-3 ± 3.00-4	4.400-3 ± 3.00-4
^{182}Ta	9	2.800-3 ± 4.00-4	4.700-3 ± 1.20-3	3.000-3 ± 1.20-3	4.700-3 ± 1.20-3
^{182}W	68	6.100-2 ± 4.00-3	6.600-2 ± 4.00-3	6.680-2 ± 6.45-3	6.600-2 ± 4.00-3
^{183}W	49	1.300-2 ± 9.00-4	1.200-2 ± 1.00-3	2.400-2 ± 2.00-3	1.300-2 ± 1.00-3
^{184}W	37	6.500-2 ± 6.00-3	8.100-2 ± 5.00-3	1.050-1 ± 2.50-2	8.100-2 ± 5.00-3
^{186}W	39	7.200-2 ± 6.00-3	8.700-2 ± 7.00-3	1.100-1 ± 2.30-2	9.000-2 ± 7.00-3
^{185}Re	477	2.920-3 ± 6.00-5	3.100-3 ± 2.00-4		3.100-3 ± 3.00-4
^{187}Re	374	3.870-3 ± 9.00-5	4.100-3 ± 3.00-4	5.000-3 ± 1.50-3	4.000-3 ± 4.00-4
^{197}Au	262	1.560-2 ± 5.00-4	1.650-2 ± 1.90-3	1.675-2 ± 1.85-3	1.650-2 ± 9.00-4
^{206}Pb	36	1.510+1 ± 1.10+0	3.570+1 ± 5.50+0		3.710+1 ± 5.50+0
^{207}Pb	12	3.800+1 ± 6.00+0	3.750+1 ± 6.50+0		3.600+1 ± 7.00+0
^{208}Pb	3	1.640+2 ± 5.20+1			1.050+2
^{209}Bi	26	3.700+0 ± 4.00-1	4.500+0 ± 6.00-1	4.895+0 ± 4.71-1	4.500+0 ± 6.00-1
^{230}Th	21	9.800-3 ± 1.10-3	9.600-3 ± 1.30-3	1.380-2 ± 5.50-3	9.600-3 ± 1.30-3
^{232}Th	241	1.650-2 ± 6.00-4	1.680-2 ± 1.00-3	1.655-2 ± 1.25-3	1.680-2 ± 1.00-3
^{231}Pa	30	4.500-4 ± 4.00-5	4.500-4 ± 5.00-5	5.500-4 ± 1.00-4	4.500-4 ± 5.00-5
^{233}Pa	33	9.900-4 ± 9.00-5	5.900-4 ± 9.00-5	6.950-4 ± 1.95-4	5.900-4 ± 9.00-5
^{232}U	12	4.200-3 ± 6.00-4	4.600-3 ± 7.00-4	5.700-3 ± 1.10-3	4.600-3 ± 7.00-4
^{234}U	118	1.180-2 ± 6.00-4	1.060-2 ± 5.00-4	1.215-2 ± 1.65-3	1.060-2 ± 5.00-4
^{235}U	232	5.100-4 ± 2.00-5	4.400-4 ± 6.00-5		4.300-4 ± 1.00-5
^{236}U	81	1.570-2 ± 9.00-4	1.470-2 ± 8.00-4	1.645-2 ± 2.55-3	1.500-2 ± 1.00-3
^{237}U	27	3.400-3 ± 3.00-4	3.500-3 ± 8.00-4		3.500-3 ± 8.00-4
^{238}U	470	2.120-2 ± 5.00-4	2.090-2 ± 1.10-3	2.230-2 ± 1.30-3	2.170-2 ± 9.00-4

Target	N_s	This Work	BNL-325	Reffo	Ignatyuk
^{237}Np	188	7.000-4 ± 3.00-5	5.200-4 ± 4.00-5	1.800-3 ± 4.00-4	5.600-4 ± 5.00-5
^{238}Np	94	6.300-4 ± 3.00-5			
^{236}Pu	20	6.300-3 ± 7.00-4			
^{238}Pu	14	8.400-3 ± 1.00-3	9.000-3 ± 7.00-4		9.000-3 ± 7.00-4
^{239}Pu	399	2.700-3 ± 1.00-4	2.300-3 ± 1.00-4	2.380-3 ± 1.80-4	2.200-3 ± 5.00-5
^{240}Pu	267	1.890-2 ± 6.00-4	1.360-2 ± 7.00-4	1.500-2 ± 1.15-3	1.240-2 ± 7.00-4
^{241}Pu	239	1.300-3 ± 4.00-5	9.000-4 ± 1.00-4	9.600-4 ± 1.60-4	7.300-4 ± 8.00-5
^{242}Pu	67	1.440-2 ± 1.00-3	1.550-2 ± 1.70-3	3.770-2 ± 2.60-3	1.330-2 ± 8.00-5
^{243}Pu	40	1.500-3 ± 1.00-4			
^{244}Pu	20	1.080-2 ± 1.30-3	1.700-2 ± 3.00-3		1.700-2
^{241}Am	190	6.000-4 ± 2.00-5	5.500-4 ± 5.00-5	6.600-4 ± 1.60-4	5.800-4 ± 4.00-5
^{242}Am	81	4.900-4 ± 2.00-5	4.000-4 ± 8.00-5	3.300-4 ± 8.00-5	4.500-4 ± 1.00-4
^{243}Am	219	6.300-4 ± 2.00-5	6.000-4 ± 6.00-5	7.700-4 ± 1.70-4	6.400-4 ± 6.00-5
^{242}Cm	12	1.860-2 ± 2.70-3	2.500-2 ± 8.00-3	2.290-2 ± 1.01-2	1.280-2 ± 2.70-3
^{243}Cm	15	5.200-4 ± 4.00-5	1.100-3 ± 2.00-4	1.300-3 ± 2.00-4	8.100-4 ± 1.00-4
^{244}Cm	37	1.100-2 ± 9.00-4	1.200-2 ± 1.00-3		1.180-2 ± 1.20-3
^{245}Cm	38	1.430-3 ± 1.20-4	1.400-3 ± 1.00-4	1.470-3 ± 1.30-4	1.380-3 ± 1.00-4
^{246}Cm	10	2.400-2 ± 3.00-3	3.400-2 ± 7.00-3	3.600-2 ± 6.00-3	3.000-2 ± 5.00-3
^{247}Cm	34	1.200-3 ± 1.00-4	1.400-3 ± 3.00-4	2.000-3 ± 1.00-4	1.400-3 ± 2.00-4
^{248}Cm	46	3.800-2 ± 3.00-3	3.300-2 ± 5.00-3	4.000-2 ± 8.00-3	2.500-2 ± 5.00-3
^{249}Bk	39	1.170-3 ± 7.00-5	1.000-3 ± 1.00-4	1.600-3 ± 2.00-4	1.000-3 ± 1.00-4
^{249}Cf	63	6.800-4 ± 3.00-5	7.000-4 ± 1.00-4	1.000-3 ± 1.00-4	7.000-4 ± 1.00-4
^{250}Cf	20	1.330-2 ± 1.60-3			
^{251}Cf	20	6.000-3 ± 6.00-4	2.700-2 ± 3.00-3		2.700-2 ± 4.00-3
^{252}Cf	20	1.700-2 ± 2.00-3			
^{253}Cf	119	5.900-4 ± 2.00-5			
^{253}Es	27	2.600-3 ± 2.00-4			

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IV DATA, PARAMETER AND PROGRAM LIBRARY

PROGRESS ON CHINESE EVALUATED NUCLEAR PARAMETER LIBRARY (CENPL) (II)

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CENPL collected, evaluated and compiled nuclear basic constants and model parameters, which are from the studies of nuclear physics for several tens of years, and made the management and retrieval by computer. It is of fundamental importance for nuclear physics. It will be very important and valuable for basic researches of nuclear physics, applications of nuclear energy and nuclear technology, and other scientifical fields (such like astrophysics and nuclear chemistry).

CENPL consists of two parts, data files and management-retrieval code system. The data files store evaluated nuclear basic constants and model

parameters according to certain format of computer which can be printed out easily with table format. The management–retrieval codes can retrieve related information for various parameters. It can also make a comparison between parameters from different authors and help users to choose and retrieve the required parameters.

The management–retrieval code system provides two retrieval ways. One is for single nucleus (SN) which retrieves related parameters for one nucleus (Z,A) only. Another is retrieval for neutron reaction (NR) which can retrieve the required parameters for target nucleus (Z,A) and the relevant residual nuclei with all possible reaction channels according to user's choose from four popular used fast neutron reaction model codes (MUP, FUP, UNF and a code including reaction processes until fourth with emissions of γ, n, p and α). The retrieved parameters will be put in an output data file with the fixed format, this output file can be used as input data file for the four type of codes mentioned above after format transformation.

CENPL–1 contains six sub–libraries, their progresses are as the following:

1 ATOMIC MASSES AND CHARACTERISTIC CONSTANTS FOR NUCLEAR GROUND STATES SUB–LIBRARY (CENPL–MCC)

MCC file contains atomic masses and mass excesses, most of them are the experimental data and the systematics results compiled by A.H.Wapstra et al.[1], the remains are the theoretical values calculated by P.Moller et al.[2] (1991 version). The total nuclear binding energy are deduced from the mass excesses. The atomic masses of exotic nuclei quite far from the valley of stability are very important for astrophysics research. The above requirement is paid attention to in our MCC file. The data for 4760 nuclides have been put into MCC file.

Most of the half–lives, spins and parities for nuclear ground states are taken from the Evaluated Nuclear Structure Data File which is the ultimate product of a data–evaluation network organized by IAEA. The others are taken from Nuclear Wallet Cards[3] (1990 version). The isotope abundances are compiled by N. E. Holden[4].

The single nucleus retrieval code has been finished in MCC sub–library. Not only the data mentioned above but also other data, which are deduced from mass excesses , can be provided by using the code system too; for example, separation energies of neutron, proton, deuteron, triton, ^{3}He, α, 2n, 2p and decay energies of β^+ and β^- decay can be obtained as the combinations of atomic masses.

2 DISCRETE LEVEL SCHEMES AND BRANCH RATIOS OF γ DECAY SUB-LIBRARY (CENPL-DLS)

One of the most time-consuming activities in nuclear model code input is the preparation of evaluated data describing the discrete level structure of all the residual nuclei involved in a complex nuclear reaction.

DLS file will begin with retrieval from the Evaluated Nuclear Structure Data File. It is important to recognize that these files contain only experimental information, which in many cases must be supplemented by evaluated data (J, π, branching ratios) in order to be used for practical cross section calculations. It is noted that CENPL will have his own format and corresponding code system for retrieving these data.

3 LEVEL DENSITY PARAMETERS SUB-LIBRARY (CENPL-LDL)

There are the following two files in LDL: experimental data file relative to level density (LRD) and level density parameters file (LDP).

LRD file includes s-wave average level spacing D_0, radioactive capture width Γ_γ^0 at neutron separation energy, and cumulative number N_0 of low-lying levels. Data for about 300 nuclides were collected and recommended by us in order to obtain two sets of new level density parameters[5, 6] for the composed four-parameter formula and back-shifted Fermi gas model in 1983 and 1987 respectively.

LDP file includes six sets of level density parameters for two popularly used level density formula, which are composed four-parameter formula and back-shifted Fermi gas formula. The first one contains the parameters of Gilbert et al.[7], Cook et al.[8] and ours[5]. The second one contains the parameters of rigid and half-rigid body of Dilg et al.[9] and ours[6]. LDP file will also contain the level density parameters of Ignatyuk et al.

Single nucleus retrieval code has been written in this sub-library. User can retrieve D_0, N_0 and Γ_γ^0 and any set of level density parameters. In order to help users to select better level density parameters, D_0 and N_0 of different level density parameters can be calculated and compared with the experimental data in LRD file by using the code system.

4 GIANT DIPOLE RESONANCE PARAMETERS FOR γ-RAY STRENGTH FUNCTION SUB-LIBRARY (CENPL-GDP)

GDP file collects the giant dipole resonance parameters of 102 nuclides from ^{51}V to ^{239}Pu, the integrated cross sections and their moments of the giant dipole resonance for photonuclear reaction of 141 nuclides from ^{1}H to ^{239}Pu compiled by Dietrich and Berman[10].

In consideration of that there are no experimental data of the giant dipole resonance parameters for some nuclei and they are necessary in practical calculations of reaction cross sections, the code system can provide the parameters required by retrieving from GDP data file with replacement, interpolation or using systematics formula respectively, according to different case.

There are two retrieval way for single nucleus (SN) and neutron reaction (NR) in the code system. The data file and code system have been finished and can be provided for using. It is needed to extend the experimental data of the giant dipole resonance parameters and to improve the systematics formula which is being studied.

5 FISSION BARRIER PARAMETER SUB-LIBRARY (CENPL-FBP)

FBP file consists of three tables: the first table contains the fission barrier parameters for 51 nuclides from ^{230}Th to ^{255}Cf recommended by Lynn[11]. The second table contains ones of 46 nuclides from ^{229}Th to ^{253}Cf obtained by Back et al.[12], through analysis of the experimental data measured by means of direct reaction in 1974. The last one comes from Ohsawa's results which are obtained in 1987 through analysis of fission cross section for 24 actinide nuclides from ^{232}Pa to ^{253}Cf.

At present, the data file and the management and retrieval code system of FBP sub-library have been finished. The code system can retrieve the fission barrier parameters for a single nucleus and the related nuclei with the (n,f), (n,nf) and (n,2nf) reaction processes. User can compare the different parameters from the three tables mentioned above, the chosen parameters or all out of them to put into the output file for using.

6 OPTICAL MODEL PARAMETERS SUB-LIBRARY (CENPL-OMP)

As the first step, the data file about the global optical model parameters for neutron and charged particle is being set up. As the complication and variousness of OMP, the file will give out the formula expressions which can be

used in optical model calculation according to the input information of the target nucleus, projectile and incoming energies and a pre–calculation with a optical model code including in this file.

The second step is setting up a data file of OMP which is used in calculations for complete neutron data in CENDL, ENDF / B–6, JENDL–3 and so on. These parameters are very important and valuable for practical application, since most of these parameters were obtained by the optimized nucleus specific OMP through fitting the updated experimental data in an energy region. Therefore we have fixed a standard optical potential form, which not only suits most popular optical potential forms but also involves the possible tendency of optical model potential development. This data file is being set up by means of dBASE method for the convenience of the format transform and output according to required format. The third step will further expand the file, in which the optical model parameters from more nuclides and more literature will be compiled.

The basic function of the management and retrieval code system for the OMP sub–library has been decided, i.e. the code system not only can retrieve the required optical model parameters, but also calculate the optical model cross section by the optical model code included in this system and compare with the experimental data.

As mentioned above a remarkable progress has been made about CENPL in the past year. There are six sub–libraries, the data file and management–retrieval code system for GDP–1 and FBP–1 have been finished. The data file and part of code system (SN retrieval) for MCC–1 and LDL–1 have been finished too. These sub–libraries have be used now, DLS and OMP are being built and some progress have been made. The next step is to finish all sub–libraries and to improve and perfect some sub–libraries further. Finally, All sub–libraries are assembled in Chinese Evaluated Nuclear Parameter Library–CENPL.

Ms. Zhang Limin, Mr. Jin Yongli, Zhao Fengquan, Sun Zhengjun, Drs. Ma Gonggui (Si Chuan University), Yao Lishan (Shaan Xi Normal University), Zhu Yaoyin (Ji Lin University) et al. take part in the above works and related activities.

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THE ESTABLISHMENT OF EXFOR NUCLEAR DATA BASE SYSTEM AND EXPERIMENTAL NEUTRON DATA LIBRARY

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Under the IAEA expert assistance, the EXFOR data base system developed by NNDC, U. S. A. has been transported to our Micro-VAX computer at CNDC.

The EXFOR data base system for experimental nuclear data consists of two parts, one is the processing code system for the nuclear data compilation in EXFOR format and format checking, another is the storage and retrieve

system, which includes two retrieval manners, i. e. on-line and batch retrieval.

Now the whole EXFOR experimental neutron data library supplied by IAEA has been loaded in the computer disk and can provide the data service to the users at any time, it is very useful and convenient to the nuclear data research work in China.

COMPUTER PROGRAM LIBRARY AT CNDC

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INTRODUCTION

With development of computer application, computer program libraries have been set up in many countries. In order to meet the needs of nuclear data calculation and nuclear energy application, Computer Program Library (CPL) at CNDC was set up in 1989. This paper covers the construction purpose and collecting fields of CPL, the judgment and category of the codes accepted by CPL.

1 PURPOSE OF CPL CONSTRUCTION

Since Chinese Nuclear Data Center was set up, more and more computer codes on theoretical calculation, evaluation and benchmark testing have been developed, collected and improved.

The importance of collecting validated nuclear model codes for calculation and evaluation of nuclear data was recognized very early indeed. The aims at minimizing costs in the development of codes and production of data, at making the best use of expert knowledge and at ensuring that users utilize them well validated, express the art methods. The task of CPL is as follows :

(1) To request codes from NEA Data Bank in order to meet the needs of the domestic users.

(2) To request codes from Chinese authors on interest shown by NEA

Data Bank. Up to now, more than 10 codes written by Chinese have been sent to NEA Data Bank. They are 19.0%[1] of total codes stored in its nuclear model program library. The percentage is less than that of USA only in the world.

(3) To collect codes from Chinese and foreigners in order to meet the needs of nuclear data calculation.

(4) To copy codes for requesters with standardized computer program package form.

(5) To collect feedback from users and transmit information between code's authors and users.

(6) To accept publications of NEA Data Bank and disseminate them to related institutes or universities in China.

2 COLLECTING FIELDS AND CATEGORY OF CODES AT CPL

The purpose to set up the Computer Program Library is to serve the nuclear data calculation, evaluation and relative nuclear energy application. So the collecting fields are limited. They are :

(1) Codes on various experimental evaluation, error analysis, data fitting and plotting;

(2) Codes on theoretical calculation of nuclear data including various theoretical models;

(3) Codes on group constant and benchmark test;

(4) Other special codes, such as mathematical routines, computer system software, codes on managing library and so on.

In order to select codes easily, the codes are classified as the following according to their function and the models they are used.

CC – Coupled Channel
DI – Direct Interaction
DWBA – Distorted Wave Born Approximation
EDP – Experimental Data Process
FKK – Feshbach–Kerman–Koonin
GMC – Generations of Multigroup Constants
INCM – Intra–nuclear Nucleon Cascade Model
OTH – Others
OM – Optical Model

PEM – Pre–Equilibrium Model
PLT – Plot
RC – Reactor Calculations
RM – R–Matrix
RP – Related Program
SM – Statistical Model
SRM – Sum Rule Model
SYS – Systematics

3 STATUS OF CPL

There are mainly two sublibraries in Computer Program Library at CNDC. One is called domestic sublibrary in which codes were written by Chinese. More than 30 codes have been put in the sublibrary, such as UNF, MUP3 and so on. Another is called foreign sublibrary in which codes originate from foreigners taken mainly through NEA Data Bank. Now there are more than 100 codes in the sublibrary and some of them are important for nuclear application in China.

In order to manage the library with computer, some codes have been developed, such as ORDEL and RETRIEVE. ORDEL is used to make index of codes. RETRIEVE can be used to retrieve codes according to code's name, category, author or keywords from code abstracts, which is similar to that of NEA Data Bank.

4 CODE EVALUATION

In order to verify the quality of these codes, first, one or two specialists are asked to check the codes on theoretical model, physical idea and calculation results. Then every code with one or more test cases supplied by the authors is compiled and excuted. Finally we organize special meeting on appraising programs to discuss on validity of model, and function of the codes to decide whether or not they are put into the library by specialists in the fields. Up to now two meetings on it have been held. The first one was in 1989 and the second in 1992. The participants are from some universities and institutes invited by CNDC.

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PROGRESS ON FREQUENTLY USEFUL NUCLEAR DECAY DATA LIBRARY

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INTRODUCTION

It is proposed to evaluate and update the frequently useful decay data for some nuclides (about 330 nuclides) for meeting Chinese users' needs. Considering their requirement, it is being done to establish the Frequently Useful Nuclear Decay Data Library at CNDC.

1 DESCRIPTION OF LIBRARY

The primary idea of constructing the Frequently Useful Nuclear Decay Data Library is as follows :

1.1 This library has comprised various decay data, which are maintained in ENSDF, NNDC, evaluated by Chinese evaluators and recommended by IAEA. It mainly contains decay data for 330 nuclides, which have been evaluated on the basis of Chinese users' requirement, decay data for x–ray and γ–ray standards for detector calibration which are recommended by IAEA, and decay data for the transactinium nuclides at present.

1.2 Users can retrieve the required decay data not only for a single nuclide but also for group nuclides simultaneously, depending on user's needs.

1.3 The ENSDF [1] format is adopted in present database.

1.4 The retrieval will be in the way of dialogue between user and computer termination.

1.5 In order to manage the library well, the code system (i. e. the retrieval program, the program TREND, by which data are shown in table, and the

program PREND, by which data are shown at scheme drawing) is expected to develop respectively and to install in relevant computer at CNDC.

2 PROGRESS

The three sorts of decay data mentioned above have been put into the Frequently Useful Nuclear Decay Data Library. Up to now, the retrieval system has been written; in addition, the TREND program and the PREND program are being transplanted and modified. The code system which combine retrieval program, the TREND program and the PREND program will be set up in near future.

3 HOW TO USE THE RETRIEVAL SYSTEM

In order to make things convenient for the users, the Menu operation is adopted, that is, users can use this retrieval program by just selecting the option in screen.

The main functions of the retrieval program are as follows :

(1) To retrieve a single nuclide or some nuclear decay data needed by user from the database.

(2) To generate table report output for these decay data.

(3) To produce scheme drawing report output for these decay data.

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V DATA PROCESSING

COVARIANCE DATA EVALUATION FOR EXPERIMENTAL DATA

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ABSTRACT

Some methods and codes have been developed and utilized for covariance data evaluation of experimental data, including parameter analysis, physical analysis, spline fitting etc.. These methods and codes can be used in many different cases.

INTRODUCTION

Recent ten years, with the developing of the reactor physics and computer technique, the covariance matrix of nuclear data becomes more and more important for nuclear engineering. For evaluators and experimenters, complete data information is given only in the case that both data themselves and their covariance matrix are given, because the errors, as traditionally given, are only the diagonal elements of the covariance matrix and describe the accuracy of the data, nothing about the correlation of the data is given. However, it is not easy to give the covariance matrix, because the matter itself is more complicated and the described methods are being developed.

Some methods and codes for covariance data evaluation of experimental data have been developed and used for last few years, including parameter analysis, physical analysis, spline function fitting etc.. They are suitable in different cases. Using these methods and codes, the experimenters or evaluators can evaluate the covariance data, calculate the covariance matrix from the uncertainty information of the experiments.

1 PARAMETER ANALYSIS

If the conditions of an experiment, especially the uncertainty information are well known, the covariance matrix can be constructed according to the formula[1]

$$\mathrm{Cov}\ (f_i,f_j)=\sum_k \frac{\partial f}{\partial x_k}\Big|_i \frac{\partial f}{\partial x_k}\Big|_j \rho_{ij}^{k}\sigma_{ki}\sigma_{kj} \tag{1}$$

$$(\text{Suppose } \rho_{ij}^{kk'}=0, \quad \text{when } k\neq k')$$

Where $\partial f/\partial x_k\,|_{i(j)}$ is the derivative of function f to parameter x_k, taken the value at $X_{ki(j)}=<X_{ki(j)}>$, $\sigma_{ki(j)}$ is the standard error of kth parameter x_k at energy point $i(j)$; and $\rho_{ij}^{kk'}$ is the correlation coefficient between parameter x_k at energy point i and parameter $x_{k'}$ at energy point j, ρ_{ij}^{k} is the correlation coefficient of parameter x_k at energy points i and j.

Form Eq. (1) it can be seen that the covariance matrix of the indirectly measured data can be constructed if its expression formula and the standard errors, the correlation coefficients of the directly measured parameters concerned are known.

In general case, it is easier for experimenters themselves to know the expression formula and the errors of the parameters. But the situation becomes more complicated for the correlation coefficients of the parameters at different energy points, which have been discussed in many papers[2~4].

If the function f or the errors Δx_k of the directly measured parameters are not known (for example for evaluators), the covariance matrix can be calculated as follows :

$$\mathrm{Cov}(f_i,f_j)=\sum_{k=1}^{N}\rho_{ij}^{k}\Delta f_{ki}\Delta f_{kj} \tag{2}$$

where, Δf_{ki} (Δf_{kj}) is the standard error of the indirectly measured data contributed from kth parameter at energy point $i(j)$. So if the partial error contributed from each parameters and their correlation coefficients at different energy points are known, the covariance matrix of indirectly measured data also can be calculated.

In mathematics, it can be proved that the constructed matrix in the way above must be symmetry and positive definite[1].

For practical application, a program CMC was developed to calculate the covariance matrix from the error information of the experiment. The calculation is performed in two cases : whether the explicit formula for the indirectly measured quantity is known. If it is known, calculation is done with formula (1) and the parameters x_{kl}, σ_{kl}, ρ_{ij}^{k} are needed to input, otherwise with formula (2) and the parameters Δf_{kl}, ρ_{ij}^{k} are needed to input. To simplify only one constant is input for some parameter if it is independent of energy.

In the explicit formula case, the subroutines for the following types of data are included:

1) Total cross section,
2) Nonelastic scattering cross section,
3) Fission cross section,
4) Activation method,
5) Capture cross section,
6) Differential cross section and spectrum with time-of-flight method.

In the implicit case, two subroutines are included :

1) The relative error of each parameters are known
2) The partial percents contributed to the total error of each parameters are known.

To insure the covariance matrix constructed is reasonable in mathematics and physics, the positive definite feature of the constructed matrix is checked by using the method of calculating the eigenvalues of the correlation coefficient matrix.

An example is given for the cross section of $^{23}Na(n,2n)^{22}Na$ reaction in the energy region from 13.0~ 18.0 MeV, measured by Lu[5] with activation method at six energy points. The measurement was carried out related to $^{93}Nb(n,2n)^{92}Nb$ cross section as standard. The calculation formula is as follows :

$$\sigma_x = \frac{N_x \left[M I_\gamma f_a f_e \varepsilon K (1 - e^{-\lambda T}) \right]_0}{N_0 \left[M I_\gamma f_a f_e \varepsilon K (1 - e^{\lambda T}) \right]_x} \tag{3}$$

where N is neutron count, M is the weight of the sample, I_γ is γ count, f_a is γ-ray correction factor in the radial direction, ε is the detector efficiency for the full energy peak, K is the correction factor for neutron flux fluctuation, and f_e is γ-ray self-absorption factor (it contributes very little, so it is neglected in the calculation). The footnote 0 and x represent the standard sample and the sample to be measured respectively.

The measured values and their errors of the quantities above at different energy points are given in table 1.

The correlation coefficients for each parameters at different energy points ρ_{ij}^{k} are given in table 2.

The calculated results are shown in table 3. The standard errors and correlation matrix are given (the error σ^{*} were given by authors).

From table 3, it can be seen that the results are reasonable :

1) The error calculated in this work are in good agreement with the ones given by the authors.

2) The correlations between first 4 points are larger, the same situation for last two points. But the correlations are smaller between first four and last two points (ρ_{15},ρ_{16},ρ_{25}, ··· etc.). This is corresponding to the situation that the measurements for first four points and last two points were completed with the same devices respectively.

2 PHYSICAL ANALYSIS

The data that their covariance is not given and the error information is not well known, which is usual case faced by the data evaluators, must be analyzed carefully in physics, and the total error, especially the main contributions for the systematic error should be found out as much as possible based on the realistic situations. Some examples, selected from the complete neutron data evaluation of Oxygen by author[6], are given as follows, which illustrate some typical cases.

2.1 Total Cross Section

In the evaluation, only one set of data[7] was taken in the energy region from 3 to 20 MeV. The information about the error given in the paper is : statistical, 0.3~1%; background correction, 1~3%; dead time < 0.1%; multi-scattering, negligible and sample error, no information. The data were normalized to their early measured data[8, 9] at 3.5 MeV. It is clear that the main systematic error comes from the normalization, which is depended on the error of their early work. But there is no exact information about the data error at 3.5 MeV, it is only known from the paper that it is less than 3%. Comparing this data around 3.5 MeV with F. G. Perey's[10] and R. B. Schrack's[11] data, it can be seen that the statistical error is 1.3% and the systematic difference between this data and Perey's data is 1.1%, which can be regarded as systematic error. So the total, used as normalization error, is 1.7%.

2.2 (n,p) Cross Section

According to the situation, as shown in Fig. 1, it is divided into three regions :

1) 16.5~20 MeV

In this region, there are two sets of data, and there are systematic differences between them. Drawing lines through each set of data, the average distance between them (divided by 2) was taken as systematic error in this region.

2) 12.6~16.5 MeV

In this region, there are 8 sets of data, but only three of them were measured in whole region, five of others only around 14 MeV, and there is no systematic difference among them. Carefully analyzing the data shows that Seeman's[12] data not only have more energy points, but also have smaller error 4% (others 8%, 10% respectively). So the curve is mainly determined by this set of data, and so the covariance. Analyzing this data shows that the total error is about 4.5% and the systematic component is 1.5% for detector efficiency and 1.0% for sample volume, so the total systematic error is 1.8%.

For convenient, a processing code CMP was written. With the code, explicit covariance matrix can be calculated and output in the ENDF / B–6 format, using the systematic error information given through above analysis in physics and the evaluated total or statistical error (for example through curve fitting), taking into account whether the systematic error needs to be added to the diagonal elements.

3 SPLINE FUNCTION FITTING

For cross section or other quantities, if there are multi–sets of measured (correlative) data and their covariance matrices are all known, the data can be fitted and the fitted values and their covariance matrix can be calculated with spline function. The fitted values

$$\hat{Y} = EY$$

and their covariance matrix

$$V_{\hat{Y}} = EV_Y E^T$$

where

$$E = B^T(W - U^T DU)$$

and Y is the vector of input measured data, V_Y is the covariance matrix of vector Y, B is base spline function matrix, and W, U, D are the matrices

concerning different weights respectively[13].

A practical program SPC was developed, by using it the multi-sets of correlative data can be fitted, and the covariance matrix of the fitted values can be calculated, which is resulted mainly from the propagation of the input covariance matrices, and also some what production in the fitting. In the program, the order of the spline function can be chosen and the spline knots can be optimized automatically[14].

Using the program, the properties of correlative data fitting and their covariance were researched. It was shown that the fitted values and their correlation coefficients are systematically changed with increasing the input correlation coefficient (suppose it is the same to all data points). Examples are given in Figs. 2~4. A practical example is given in Fig. 1, which was taken from the evaluation of Oxygen complete data for CENDL-2.

It was also found that the PPP problem[15] happened when the data to be fitted are in large discrepancy and the correlation is strong (see Fig. 2, curves No. 5, 6). In this case, the fit values are outside the input experimental data and are not reasonable. To solve this problem, the input absolute covariance matrix is iterated, keeping the input relative covariance matrix unchanged and replacing the input experimental data by fit values. An example is given in Fig. 5, the start curve is the curve No. 6 in Fig. 2. As a practical example, the change of output covariance matrix with iteration is given in Fig. 6.

CONCLUSION REMARKS

The methods and codes for covariance data evaluation of experimental data described above can be used in different cases and for different purpose. The parameter analysis can be used for experimenters to construct the covariance matrix of their measured data, because they well know the experiment conditions, especially the information about the error. The evaluators usually have to do physical analysis, because they face large amount of data and not well know the measurement conditions. The spline fit is suitable for both experimenters and evaluators to process their correlative data : calculate the fit values and their covariance matrix, but it can be used only in the case that the covariance matrices of input data are all already known.

Table 1 The measured values and their standard errors of the quantities concerned

quan.	E_n = 13.5 MeV		E_n = 14.1 MeV		E_n = 14.64 MeV	
	Value	error	Value	error	Value	error
N_s	3.85×10^{-3}	0.92%	1.1825×10^{-2}	1.2%	2.5259×10^{-2}	0.43%
M_o	2.01882×10^{21}	0.2%	1.6409×10^{21}	0.2%	1.3553×10^{21}	0.2%
I_{ys}	0.990		0.990		0.990	
f_{so}	0.995	0.1%	0.996	0.1%	0.998	0.1
ε_o	0.03248	1.2%	0.03248	1.2%	0.03248	1.2%
K_o	1.0147	0.1%	1.0147	0.1%	1.0147	0.1%
$(1-e)_o^{-\lambda T}$	0.2365		0.2365		0.2365	
σ_o	448	7.4	456.7	4.7	459	5.0
N_o	90.22	0.5%	69.602	0.5%	64.690	0.5%
M_s	3.1769×10^{22}	0.4%	3.0507×10^{22}	0.4%	2.9441×10^{22}	0.4%
I_{ys}	0.9994		0.9994		0.9994	
f_{ss}	0.9635	0.4%	0.9650	0.4%	0.9664	0.4%
ε_s	0.0005783	0.8%	0.0005783	0.8%	0.0005793	0.8%
$(1-e)_s^{-\lambda T}$	2.8773×10^{-3}		2.8773×10^{-3}		2.8773×10^{-3}	

quan.	E_n = 14.87 MeV		E_n = 16.95 MeV		E_n = 17.98 MeV	
	Value	error	Value	error	Value	error
N_s	3.0235×10^{-2}	0.7%	0.1231	0.36%	0.2822	0.26%
M_o	1.1914×10^{21}	0.2%	6.4818×10^{18}	0.2%	6.4818×10^{18}	0.2%
I_{ys}	0.990		0.990		0.990	
f_{so}	0.998	0.1%	0.998	0.1%	0.996	0.1
ε_o	0.03248	1.2%	0.03248	1.2%	0.03248	1.2%
K_o	1.0147	0.1%	0.9911	0.1%	0.9933	0.1%
$(1-e)_o^{-\lambda T}$	0.2365		0.1644		0.1043	
σ_o	4	6.0	413	11.0	388	15.0
N_o	57.612	0.5%	0.04729	0.5%	0.09549	0.5%
M_s	3.3073×10^{22}	0.4%	1.4342×10^{22}	0.4%	1.4342×10^{22}	0.4%
I_{ys}	0.9994		0.9994		0.9994	
f_{ss}	0.9623	0.4%	0.9869	0.4%	0.9840	0.4%
ε_s	0.0005783	0.8%	0.01509	0.8%	0.01509	0.8%
$(1-e)_s^{-\lambda T}$	2.8773×10^{-3}		1.9163×10^{-3}		1.1754×10^{-3}	

Table 2 The correlation coefficients of directly measured quantities

Measured quantities	Correlation coefficient	Comments
x_k	f_{ij}^k	
N_s	0	completely
N_o	0	statistical
M_s	1.0	completely
M_o	1.0	systematical
ε_o	1.0	
f_{ss}	0.7	statistical and systematical,
f_{so}	0.7	mainly systematical
σ_o	0.5	estimate
ε_s	1.0, i, j= 1~4 or 5,6	same device
	0.7 i= 1~4, j= 5,6	different device

Table 3 The correlation matrix and standard error for ^{23}Na(n,2n) reaction (ρ)

E_n	E_n (MeV)					
	13.5	14.10	14.64	14.87	16.95	17.98
13.50 MeV	1.0000					
14.10 MeV	0.5543	1.0000				
14.64 MeV	0.6398	0.6281	1.0000			
14.87 MeV	0.6423	0.6201	0.7140	1.0000		
16.95 MeV	0.5094	0.4390	0.5122	0.5325	1.0000	
17.98 MeV	0.4720	0.3897	0.4571	0.4834	0.5435	1.0000
σ	0.14	0.45	0.78	0.87	2.69	4.05
σ^*	0.16	0.50	0.80	0.90	3.0	4.3

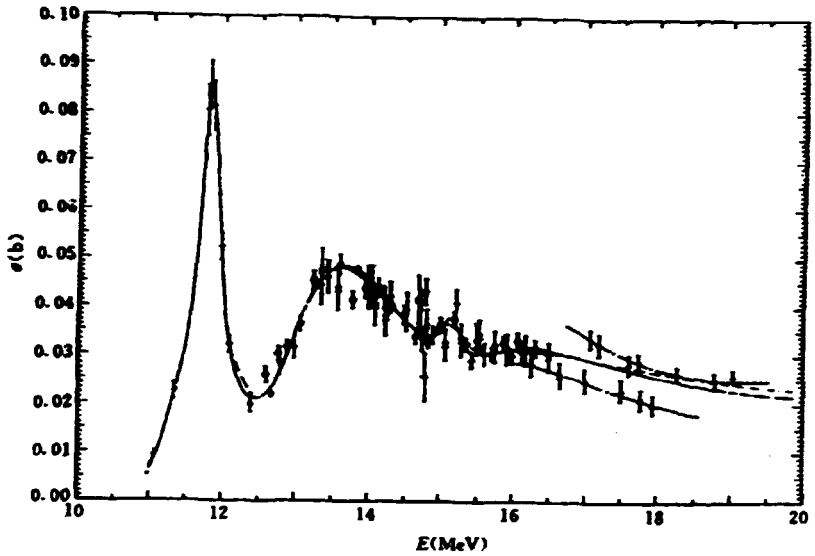

Fig. 1 O(n,p) cross section

● etc. exp. data; —— fit curve, $\rho=0.0$; – – – fit curve, $\rho=0.5$;
— · — The line to estimate the systematic error in the energy region 16.5 to 20 MeV.

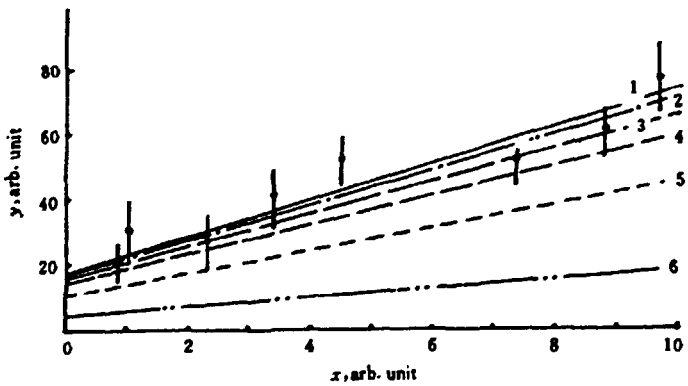

Fig. 2 The changing of fit values with the correlation coefficient ρ of input data
1 $\rho=0.0$; 2 $\rho=0.2$; 3 $\rho=0.4$; 4 $\rho=0.6$; 5 $\rho=0.8$; 6 $\rho=0.95$.

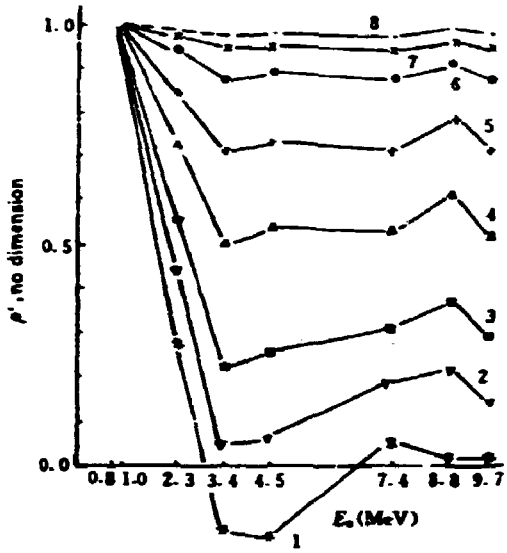

Fig. 3 The effect of the input correlation coefficient ρ on the correlation coefficient ρ' of fit values

1 $\rho=0.0$; 2 $\rho=0.1$; 3 $\rho=0.2$; 4 $\rho=0.4$;
5 $\rho=0.6$; 6 $\rho=0.8$; 7 $\rho=0.9$; 8 $\rho=0.95$.

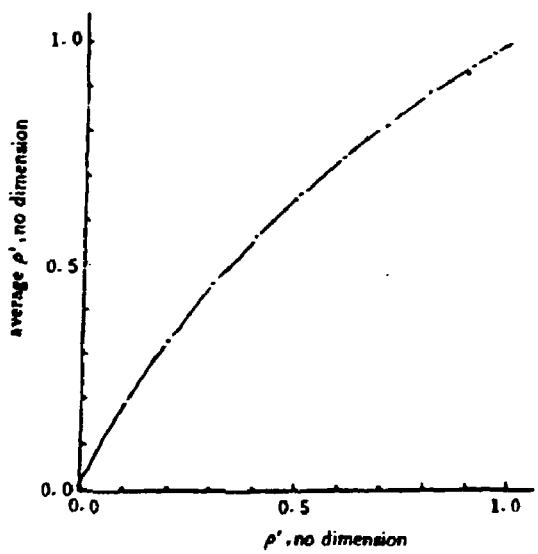

Fig. 4 The changing of average correlation coefficient ρ' of fit values with input correlation coefficient ρ

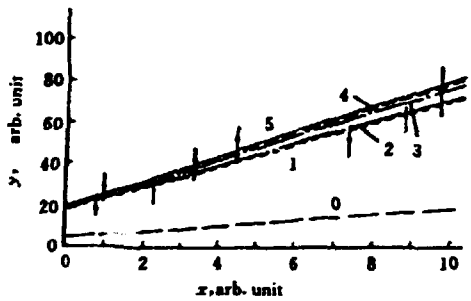

Fig. 5 The changing of fit values with iteration

The numbers in the figure are the iteration times

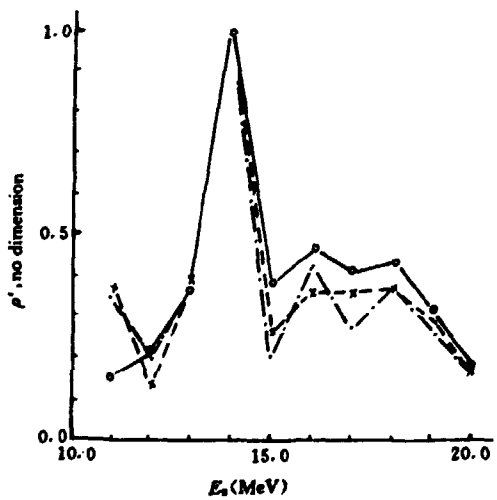

Fig. 6 The effecting of iteration times k on the correlation coefficient ρ' of fit values for O(n,p) cross section

× $k=0$; ○ $k=1$; · $k=2$.

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SEVERAL EXAMPLES OF LEAST SQUARES COMBINATION FOR DERIVED DATA

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INTRODUCTION

"Peelle's Pertinent Puzzle (PPP)" was posed by R. W. Peelle in 1987[1]. In the past five years, many individuals have been involved in the discussion on this puzzle[2] and several publications presented[3~7].

In author's opinion[3, 4], the PPP was attributed to the inconsistencies in generating derived quantities and their covariance matrix from directly measured data associated with their uncertainties through non-linear relation and PPP can be solved by eliminating the inconsistencies through an iterative procedure. Recently, R. L. Perel et al. presented their argument on PPP. They wrote in their paper[7]: "There is no need to fall back on the non-linearity of X". They presented the formalism for data combination in their paper and declared that by using their formalism the Peelle's example have been solved.

In this work, three examples including Peelle's example for the combination of the derived data are calculated by using the formalism given by Perel et al.. In first example, the derived data are generated through two linear and different relations. The two estimates, calculated by Perel's formalism in two equivalent ways, are consistent with each other and also consistent with the right least square estimate we declared. In this example, the estimate reasonablely falls outside the data range. In second and third examples, the derived data to be combined are generated from directly measured data through non-linear relations, the two estimates, obtained by using Perel's formalism in two equivalent ways, neither consistent with each other nor consistent with right least square estimate we declared. The details of calculation are given in the next Section of this paper.

1 COMPUTATIONAL EXAMPLES

In the following examples,same symbols as in Perel's paper are used. All of

directly measured data are considered to be independent with each other, so that $C_{pr} = 0$.

1.1 Linear Relation

We are given three independent directly measured data

$$a_1 = 2.5 \pm 0.15 \quad b_1 = 5/3 \pm 0.10 \quad m_1 = 1.0 \pm 0.30 \tag{1}$$

and two relations

$$y_1 = a_1 - m_1 \qquad y_2 = b_1 - 2m_1/3 \tag{2}$$

What are the least square estimates for $<y>$, $<a>$, $<b>$ and $<m>$?

Our solutions for this examples can be found in example 5.1 of Ref. [3] and summaried in table 1.

Table 1 Zhao's results of example 1

Estimate	Std. Dev.	Correlation Matrix			
$\hat{y} = 0.8823$	0.2183	1.00			
$\hat{a} = 2.2353$	0.1029	−0.23	1.00		
$\hat{b} = 1.7842$	0.0875	0.65	0.59	1.00	
$\hat{m} = 1.3529$	0.2623	−0.92	0.59	−0.31	1.00

Perel's formalism can be used to solve this problem in two equivalent ways.

WAY 1 : Starting from

$$P_1 = a_1 - m_1 = 1.5; \quad P_2 = a_1 = 2.5; \quad P_3 = m_1 = 1.0 \tag{3}$$

$$C_p = \begin{bmatrix} \sigma^2(a_1) + \sigma^2(m_1) & & \\ \sigma^2(a_1) & \sigma^2(a_1) & \\ -\sigma^2(m_1) & 0 & \sigma^2(m_1) \end{bmatrix} = \begin{bmatrix} 0.1125 & & \\ 0.15^2 & 0.15^2 & \\ -0.3^2 & 0 & 0.3^2 \end{bmatrix} \tag{4}$$

$$r = b_1 = 5/3 \qquad C_r = 0.1^2 \tag{5}$$

we have

$$\bar{r} = b = P_1 + 2P_3/3 = 2.1667 \qquad d = \bar{r} - r = 0.5 \tag{6}$$

$$S = \left[\frac{\partial \bar{r}}{\partial P_1} \quad \frac{\partial \bar{r}}{\partial P_2} \quad \frac{\partial \bar{r}}{\partial P_3} \right] = [1 \quad 0 \quad 2/3] \tag{7}$$

$$C_d = SC_p S^T + C_r = 0.0425 \tag{8}$$

$$P' = P - C_p S^T C_d^{-1} d = \begin{bmatrix} 0.8823 \\ 2.2353 \\ 1.3529 \end{bmatrix} \tag{9}$$

$$C_{p'} = C_p - C_p S^T C_d^{-1} S C_p = \begin{bmatrix} 0.04765 & & \\ -0.00529 & 0.01059 & \\ -0.05294 & 0.01588 & 0.06882 \end{bmatrix} \tag{10}$$

$$r' = r + C_r C_d^{-1} d = 1.7842 \tag{11}$$

$$C_{r'} = C_r - C_r C_d^{-1} C_r = 0.007647 \tag{12}$$

$$C_{p'r'} = C_p S^T C_d^{-1} C_r = \begin{bmatrix} 0.01235 \\ 0.00529 \\ -0.00706 \end{bmatrix} \tag{13}$$

Remembering that

$$P'_1 = \hat{y} \quad P'_2 = \hat{a} \quad P'_3 = \hat{m} \quad r' = \hat{b} \tag{14}$$

the results above are exactly consistent with those in table 1.

WAY 2:

Now, let us start from

$$P_1 = b_1 - 2m_1/3 = 1.0 \quad P_2 = b_1 = 5/3$$
$$P_3 = m_1 = 1.0 \quad r = a_1 = 2.5 \tag{15}$$

same results with those from WAY 1 can be obtained.

1.2 Non-linear Relation (Peelle's example)

We are given three independent directly measured data

$$a_1 = 1.0 \pm 0.10 \quad a_2 = 1.5 \pm 0.15 \quad m_1 = 1.0 \pm 0.20 \tag{16}$$

and non–linear relation

$$y = a / m \tag{17}$$

What are the least square estimates for $<y>$, $<a>$ and $<m>$?

Our solutions for this examples were given in example 5.2 of Ref. [3] and summaried in table 2a.

Table 2a Zhao's results of example 2

Estimate	Std. Dev.	Correlation Matrix		
$\hat{y} = 1.1538$	0.2453	1.00		
$\hat{a} = 1.1538$	0.0832	0.34	1.00	
$\hat{m} = 1.0000$	0.2000	−0.94	0.00	1.00

Let us use Perel's formalism to this problem.

WAY 1: Starting from

$$P_1 = a_1 / m_1 = 1.0 \qquad P_2 = m_1 = 1.0 \tag{18}$$

$$C_p = \begin{bmatrix} \sigma^2(a_1)/m_1^2 + a_1^2\sigma^2(m_1)/m_1^4 & \\ -a_1\sigma^2(m_1)/m_1^2 & \sigma^2(m_1) \end{bmatrix} = \begin{bmatrix} 0.05 & \\ -0.04 & 0.04 \end{bmatrix} \tag{19}$$

$$r = a_2 = 1.5 \qquad C_r = 0.0225 \tag{20}$$

we have

$$\bar{r} = P_1 P_2 = 1.0 \quad d = \bar{r} - r = -0.5 \tag{21}$$

$$S = \begin{bmatrix} \frac{\partial \bar{r}}{\partial P_1} & \frac{\partial \bar{r}}{\partial P_2} \end{bmatrix} = \begin{bmatrix} P_2 & P_1 \end{bmatrix} = \begin{bmatrix} 1.0 & 1.0 \end{bmatrix} \tag{22}$$

$$C_d = S C_p S^T + C_r = 0.0325 \tag{23}$$

$$P' = P - C_p S^T C_d^{-1} d = \begin{bmatrix} 1.1538 \\ 1.0000 \end{bmatrix} \tag{24}$$

$$C_{p'} = C_p - C_p S^T C_d^{-1} S C_p = \begin{bmatrix} 0.04692 & \\ -0.04 & 0.04 \end{bmatrix} \tag{25}$$

$$r' = r + C_r C_d^{-1} d = 1.1538 \tag{26}$$

$$C_{r'} = C_r - C_r C_d^{-1} C_r = 0.0832^2 \tag{27}$$

$$C_{pr'} = C_p S^T C_d^{-1} C_r = \begin{bmatrix} 0.0832^2 \\ 0 \end{bmatrix} \tag{28}$$

Remembering that

$$P'_1 = \hat{y} \quad P'_2 = \hat{m} \quad r' = \hat{a} \tag{29}$$

the results above are summaried in table 2b. The item denoted by "?" in table 2b are different from those in table 2a.

Table 2b Results of WAY 1 by Perel's formalism for example 2

Estimate	Std. Dev.	Correlation Matrix		
$\hat{y} = 1.1538$	0.2166?	1.00		
$\hat{a} = 1.1538$	0.0832	0.38?	1.00	
$\hat{m} = 1.0000$	0.2000	−0.92?	0.00	1.00

WAY 2:

Now, let us start from

$$P_1 = a_2 = 1.5 \quad P_2 = m_1 = 1.0 \quad r = a_1 = 1.0 \tag{30}$$

we have

$$C_p = \begin{bmatrix} 0.1125 & \\ -0.06 & 0.04 \end{bmatrix} \quad C_r = 0.01 \tag{31}$$

$$\bar{r} = P_1 P_2 = 1.5 \quad d = \bar{r} - r = 0.5 \quad C_d = 0.0325 \tag{32}$$

$$S = \left[\frac{\partial \bar{r}}{\partial P_1} \quad \frac{\partial \bar{r}}{\partial P_2} \right] = \left[P_2 \quad P_1 \right] = \left[1.0 \quad 1.5 \right] \tag{33}$$

$$P' = \begin{bmatrix} 1.1538 \\ 1.0000 \end{bmatrix} \quad C_{P'} = \begin{bmatrix} 0.09692 & \\ -0.06 & 0.04 \end{bmatrix} \tag{34}$$

$$r' = 1.1538 \quad C_{r'} = 0.0832^2 \quad C_{P'r'} = \begin{bmatrix} 0.006923 \\ 0 \end{bmatrix} \tag{35}$$

The results above are summaried in table 2c. These results are neither consistent with Zhao's nor consistent with those from WAY 1.

Table 2c Results of WAY 2 by Perel's formalism for example 2

Estimate	Std. Dev.	Correlation Matrix		
$\hat{y} = 1.1538$	0.3113?	1.00		
$\hat{a} = 1.1538$	0.0832	0.27?	1.00	
$\hat{m} = 1.0000$	0.2000	−0.96?	0.00	1.00

1.3 Non-linear Relation (No Correlation Between Derived Data)

We are given two independent directly measured data

$$a_1 = 1.0 \pm 0.10 \qquad a_2 = 1.5 \pm 0.15 \tag{36}$$

and non-linear relation

$$y = a^2 \tag{37}$$

What are the least square estimates for $<y>$, $<a>$?

Right solutions for this example can be obtained as follows :

$$\hat{a} = \frac{a_1 / \sigma^2(a_1) + a_2 / \sigma^2(a_2)}{1/\sigma^2(a_1) + 1/\sigma^2(a_2)} = 1.1538 \tag{38}$$

$$\sigma^2(\hat{a}) = (1/\sigma^2(a_1) + 1/\sigma^2(a_2))^{-1} = 0.0832^2 \tag{39}$$

$$\hat{y} = \hat{a}^2 = 1.3313 \qquad \sigma^2(\hat{y}) = (2\hat{a})^2\sigma^2(\hat{a}) = 0.1920^2$$
$$\mathrm{Cov}(\hat{y},\hat{a}) = 2\hat{a}\sigma^2(\hat{a}) = 0.01597 \tag{40}$$

The results above are summaried in table 3a.

Table 3a Zhao's results of example 3

Estimate	Std. Dev.	Correlation Matrix	
$\hat{y} = 1.3313$	0.1920	1.00	
$\hat{a} = 1.1538$	0.0832	1.00	1.00

Let us use Perel's formalism to this problem.

WAY 1: Starting from

$$P = a_1^2 = 1.0 \qquad C_p = 4a_1^2\sigma^2(a_1) = 0.04 \tag{41}$$

$$r = a_2 = 1.5 \qquad C_r = 0.15^2 \tag{42}$$

we have

$$\bar{r} = a_1 = 1.0 \qquad d = \bar{r} - r = -0.5 \tag{43}$$

$$S = \frac{\partial \bar{r}}{\partial p} = \frac{1}{2a_1} = 0.5 \qquad C_d = 0.0325 \tag{44}$$

$$P' = 1.3077 \qquad C_{p'} = 0.1664^2 \qquad r' = 1.1538 \tag{45}$$

$$C_{r'} = 0.0832^2 \qquad C_{p'r'} = 0.01385 \tag{46}$$

Remembering that

$$P' = \hat{y}; \qquad r' = \hat{a} \tag{47}$$

the results above are summaried in table 3b.

Table 3b Results of WAY 1 by Perel's formalism for example 3

Estimate	Std. Dev.	Correlation Matrix	
$\hat{y}$ = 1.3077?	0.1664?	1.00	
$\hat{a}$ = 1.1538	0.0632	1.00	1.00

WAY 2:

Now, let us start from

$$P = a_2^2 = 1.5^2 \qquad r = a_1 = 1.0 \tag{48}$$

we have

$$C_p = 4a_2^2\sigma^2(a_2) = 0.2025 \qquad C_r = 0.01 \tag{49}$$

$$\bar{r} = 1.5 \qquad d = \bar{r} - r = 0.5 \tag{50}$$

$$S = \frac{\partial \bar{r}}{\partial P} = \frac{1}{2a_2} = 1/3 \qquad C_d = 0.0325 \tag{51}$$

$$P' = 1.2115 \qquad C_{p'} = 0.2496^2 \tag{52}$$

$$r' = 1.1538 \qquad C_{r'} = 0.0832^2 \qquad C_{p'r'} = 0.02077 \tag{53}$$

The results above are summaried in table 3c.

Table 3c Results of WAY 2 by Perel's formalism for example 3

Estimate	Std. Dev.	Correlation Matrix	
$\hat{y}$ = 1.2115	0.2496?	1.00	
$\hat{a}$ = 1.1538	0.0832	1.00	1.00

With comparison among Table 3a,3b and 3c, it can be seen that the results

for derived data from Perel's formalism are neither consistent with right one nor consistent between two equivalent ways.

2 CONCLUDING REMARK

From the computational examples above it would be clear that Perel's formalism only work in the linear situation. The fact that the estimates for derived data and their covariance matrix calculated from Perel's formalism in non-linear situations are neither consistent with right one we declared nor self consistent demonstrates that consistence problem must be noticed in generating derived data and their covariance matrix from directly measured data through non-linear relation.Failure to recognize such an implication can led to inconsistency between the results of different evaluation strategies. This is just what we learnt from PPP.

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VI THERMAL NEUTRON SCATTERING LAW

CALCULATION OF THERMAL NEUTRON SCATTERING LAW FOR ANISOTROPIC MICROCRYSTAL

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ABSTRACT

A method of calculating thermal neutron scattering law for anisotropic microcrystal which is based on Fourier transform is derived in this paper. A formula for Debye–Waller factor is derived, too. Results of anisotropic graphite scattering law by the code SCAT–3 based on the method are presented. It is shown that the method is accurate and efficient and that it is very important to take a correct value of Debye–Waller factor.

INTRODUCTION

It is well known that in the incoherent approximation the double scattering cross section can be expressed in the form.

$$\sigma(E_o \to E,\mu) = \frac{\sigma_b}{4\pi}\left(\frac{E}{E_o}\right)^{1/2} e^{-\beta/2} S(\alpha,\beta) = \frac{\sigma_b}{4\pi}\left(\frac{E}{E_o}\right)^{1/2} \mathcal{S}(\alpha,\beta) \qquad (1)$$

where $\mathcal{S}(\alpha,\beta)$ is an explicit function called the scattering law of two variables α and β defined as

$$\alpha = \frac{\bar{k}^2}{2MT} = \frac{E_o + E - 2\mu\sqrt{E_o E}}{MT}, \quad \beta = \frac{E}{T} = \frac{E_o - E}{T} \tag{2}$$

where $\bar{k}$ and E are the neutron momentum and energy exchanges respectively, M is the atomic mass of main scatterer, T is the temperature, and σ_b is the bound atom scattering crass section. The Fourier transform $\chi(\alpha, t)$ (called intermediate scattering function) of the scattering law

$$\chi(\alpha,t) = \int_{-\infty}^{\infty} \exp\ (\ \imath Et\ )\ S\ (\alpha,\beta)\ \mathrm{d}E \tag{3}$$

is the product of the partial χ– functions

$$\chi(\alpha,t) = \prod_i \chi_i\ (\alpha,t) \tag{4}$$

here $\chi_i(\alpha,t)$ is a basic intermediate scattering function which is exponential in α :

$$\chi_i\ (\alpha,t) = \exp\ [\ \alpha\ W_i\ G_i\ (t)\ ] \tag{5}$$

The basic intermediate scattering functions include the following dynamical modes of the scatter :

1. Free translation;
2. Diffusive or Brownian motion;
3. Harmonic isotropic vibrations with continuous frequency spectrum;
4. Harmonic anisotropic vibrations with continuous frequency spectrum;
5. Harmonic isotropic vibrations with discrete frequency spectrum.

Koppel J. U. et al. developed GASKET code[1] which only includes above modes 1 ~ 3, 5. They made an attempt to include the mode 4, but they met some difficulties in deriving formulas. GASKET (and GASKET–II) didn't overcome the difficulties. So they had to use isotropic vibrations with continuous frequency spectrum mode 3 instead of anisotropic vibrations with continuous frequency spectrum mode 4 as applied to graphite for instance.

A method of calculating thermal neutron scattering law for anisotropic vibrations with continuous frequency spectrum and its combinations with other modes is derived herein.

1 ANISOTROPIC VIBRATION MODE AND ITS COMBINATION WITH OTHER MODES

A. Harmonic anisotropic vibrations with continuous frequency spectrum

For harmonic anisotropic vibrations with continuous frequency spectrum, it is possible to introduce an orientation–dependent frequency spectrum of the form

$$f(\omega) = f_{\parallel}(\omega)\,\mu^2 + f_{\perp}(\omega)\,(1-\mu^2) \tag{6}$$

where μ is the angle cosine between a preferred direction in the microcrystal and a fixed axis which is parallel to the momentum exchange $\bar{k}$, $f_{\perp}(\omega)$ and $f_{\parallel}(\omega)$ are the frequency spectra associated with modes having polarization vectors which are perpendicular and parallel to the preferred direction respectively.

We note that at μ the function $\chi(\alpha, t, \mu)$ is the product of $\chi_{\perp}(\alpha, t, \mu)$ and $\chi_{\parallel}(\alpha, t, \mu)$.

$$\chi(\alpha,t,\mu) = \chi_{\perp}(\alpha,t,\mu) \cdot \chi_{\parallel}(\alpha,t,\mu) \tag{7}$$

where $\chi_{\perp}(\alpha,t,\mu)$ and $\chi_{\parallel}(\alpha,t,\mu)$ are perpendicular and parallel partial χ – functions. Calculation of $\chi_{\perp}(\alpha, t,\mu)$ or $\chi_{\parallel}(\alpha, t,\mu)$ is similar to χ – functions for harmonic isotropic vibration. In fact we get[2, 3]

$$\chi_{\perp}(\alpha,t,\mu) = \exp\left[\, G_{\perp}(t)\,\alpha\, W_4\,(1-\mu^2)\,\right] \tag{8}$$

$$\chi_{\parallel}(\alpha,t,\mu) = \exp\left[\, G_{\parallel}(t)\,\alpha\, W_4\,\mu^2\,\right] \tag{9}$$

where

$$G_{\perp}(t) = \gamma_{\perp}(t) - \gamma_{\perp}(0) \tag{10}$$

$$\gamma_{\perp}(t) = \frac{1}{W_4}\left[\, H_{\perp}(t) + i\, F_{\perp}(t)\,\right] \tag{11}$$

$$H_{\perp}(t) = W_4 T \int_0^{W_{max}} f_{\perp}(\omega) \coth\left(\frac{\omega}{2T}\right) \cos \omega t \, \frac{d\omega}{\omega} \tag{12}$$

$$F_{\perp}(t) = W_4 T \int_0^{W_{max}} f_{\perp}(\omega) \sin \omega t \frac{d\omega}{\omega} \tag{13}$$

$$G_{\perp}(t)\alpha W_4 = \alpha [H_{\perp}(t) - H_{\perp}(0)] + i \alpha F_{\perp}(t) \tag{14}$$

$G_{//}(t)$, $\gamma_{//}(t)$, $H_{//}(t)$, $F_{//}(t)$ can be got similarly.
Substitute these to (7), (8) and (9), we get[2]

$$\chi(\alpha,t,\mu) = \exp \{ \alpha (H_{\perp} - H_{\perp,0} + i F_{\perp}) \} \cdot \exp \{ -\alpha \mu^2 (H_{\perp} - H_{\perp,0} - H_{//} + H_{//,0}) - i \alpha \mu^2 (F_{\perp} - F_{//}) \} \tag{15}$$

(Hereinafter, $H_{\perp}$ replaces $H_{\perp}(t)$, $H_{\perp}$, 0 replaces $H_{\perp}(0)$, etc.)
Here we note that $\chi(\alpha, t,\mu)$ is complex, because $r_{\perp}(t)$ and $r_{//}(t)$ are complex.
We get integral[2].

$$\chi_4(\alpha,t) = \int_0^1 d\mu \, \chi(\alpha,t,\mu) = \exp \{ \alpha [H_{\perp} - H_{\perp,0}] \} \cdot \{ [\cos (\alpha F_{\perp}) EC(t) - \sin (\alpha F_{\perp}) \cdot ES(t)] + i [\sin (\alpha F_{\perp}) \cdot EC(t) + \cos (\alpha F_{\perp}) \cdot ES(t)] \} \tag{16}$$

where

$$EC(t) = \int_0^1 d\mu \cos [(F_{//} - F_{\perp}) \alpha \mu_2] \cdot \exp [(H_{//} - H_{\perp} - H_{//,0} + H_{\perp,0}) \alpha \mu^2] \tag{17}$$

$$ES(t) = \int_0^1 d\mu \sin [(F_{//} - F_{\perp}) \alpha \mu_2] \cdot \exp [(H_{//} - H_{\perp} - H_{//,0} + H_{\perp,0}) \alpha \mu^2] \tag{18}$$

Do the Fourier inversion of Eq. (16), we get[2].

$$S_{,}(\alpha,\beta) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dt \, e^{iEt} \cdot \exp \{ \alpha (H_{\perp} - H_{\perp,0}) \} \cdot \{ \cos (\alpha F_{\perp}) EC(t) - \sin (\alpha F_{\perp}) ES(t) + i [\sin (\alpha F_{\perp}) EC(t) + \cos (\alpha F_{\perp}) ES (t)] \}$$

$$= \frac{D_\perp}{\pi} \int_0^\infty dt \{ \cos(Et) [\cos(\alpha F_\perp) EC(t) - \sin(\alpha F_\perp) ES(t)] - \sin(Et) [\sin(\alpha F_\perp) EC(t) + \cos(\alpha F_\perp) ES(t)] \} e^{\alpha H_\perp} \quad (19)$$

where

$$D_\perp = \exp\{ -\alpha W_4 \gamma_\perp(0) \} = \exp\{ -\alpha H_{\perp,0} \} \quad (20)$$

Right–hand of Eq. (17) and (18) are evaluated by Guass–Sidel integral formula with grade 8 or so.

B. χ – function of anisotropic crystals

χ–function of anisotropic crystals for example graphite, is a combination of mode 4 and mode 1. Nearby μ we have.

$$\chi_{1-4}(\alpha,t,\mu) = \chi_1(\alpha,t)\, \chi_4(\alpha,t,\mu) = \exp(-\alpha W_1 T^2 t^2 + i \alpha W_1 T t) \cdot \exp\{ -\alpha H_{\perp,0} + \alpha\mu^2 (H_{\perp,0} - H_{\parallel,0}) \} \cdot \exp\{ \alpha H_\perp + i \alpha F_\perp + \alpha\mu^2 [H_\parallel - H_\perp + i (F_\parallel - F_\perp)] \} \quad (21)$$

It is very important to separate from χ– function the term which corresponds to zero–phonon scattering. So we have the following expressions[2]

$$\chi_{1-4}(\alpha,t,\mu) = \chi_1(\alpha,t) \{ \chi_4(\alpha,t,\mu) - D(\mu) \} + D(\mu)\, \chi_1(\alpha,t) \quad (22)$$

$$D(\mu) = \exp\{ -\alpha H_{\perp,0} + \alpha\mu^2 (H_{\perp,0} - H_{\parallel,0}) \} = D_\perp \cdot \exp\{ \alpha\mu^2 (H_{\perp,0} - H_{\parallel,0}) \} \quad (23)$$

$$D_\perp = \exp(-\alpha H_{\perp,0}) \quad (24)$$

To integrate Eq. (22), we get.

$$\chi_{1-4}(\alpha,t) = \chi_1(\alpha,t) \{ \chi_4(\alpha,t) - \bar{D} \} + \bar{D} \chi_1(\alpha,t) \quad (25)$$

where

$$\bar{D} = \int_0^1 d\mu\, D(\mu) = D_\perp \int_0^1 d\mu \exp\{\alpha\mu_2 (H_{\perp,0} - H_{\parallel,0})\} \quad (26)$$

$\bar{D}$ is the so-called Debye-Waller factor which we search for. Then, the inverse Fourier transform to $\chi_{1-4}(\alpha,t)$ is

$$S_{1-4}(\alpha,\beta) = \frac{D_\perp}{\pi} \int_0^\infty dt\, [\, Q_4(t) \cos \lambda t - R_4(t) \sin \lambda t\,] + \bar{D} S_1(\alpha,\beta) \quad (27)$$

where

$$\lambda = E + \alpha T W_1 = (\beta + \alpha W_1) T \quad (28)$$

$$\theta_4(t) = \{[\cos(\alpha F_\perp) EC(t) - \sin(\alpha F_\perp) \cdot ES(t)] \cdot \exp(\alpha H_\perp) - \frac{\bar{D}}{D_\perp}\} \cdot \exp\{-\alpha W_1 T^2 t^2\} \quad (29)$$

$$R_4(t) = [\sin(\alpha F_\perp) \cdot EC(t) + \cos(\alpha F_\perp) \cdot ES(t)] \exp\{\alpha H_\perp - \alpha W_1 T^2 t^2\} \quad (30)$$

$$S_1(\alpha,t) = \frac{e^{-\beta/2}}{\sqrt{4\pi\alpha W_1 T^2}} \cdot \exp\left[-\frac{1}{4\alpha W_1}(\beta^2 + \alpha^2 W_1^2)\right] \quad (31)$$

where $EC(t)$ and $ES(t)$ are given by Eq. (17) and Eq. (18) separately. $\bar{D}$ is given by Eq. (26) which is evaluated by Guass-Sidel integral formula with grade 8 or so.

It is found that only to use the correct value $\bar{D}$ by Eq. (26) may Eq. (27) converge. Otherwise Eq. (27) disconverges[2].

2 RESULTS

The code SCAT-3 based on above method has been used in calculation for scattering of anisotropic crystal. And some results about anisotropic crystal of

graphite are presented herein.

A. Comparison between anisotropic and isotropic modes

Results for scattering law of graphite in anisotropic mode are presented in table 1 (the third line) and in Fig. 1 (the unbroken curve). And results in isotropic approximate mode are also presented in table 1 (the second line) and in Fig. 1 (the dotted curve). In isotropic approximation, the frequency spectrum is obtained by.

$$f(\omega) = \frac{1}{4\pi} \int_{\Omega} f(\omega,\bar{\Omega})\, d\Omega = \int_0^1 f(\omega,\mu)\, d\mu$$
$$= \frac{1}{3} f_{//}(\omega) + \frac{2}{3} f_{\perp}(\omega) \tag{32}$$

Comparing isotropic approximation with anisotropic mode we find that the scattering law as result of isotropic approximation approaches the one of anisotropic mode roughly. Isotropic approximation by Eq. (32) has certain precision. But in some cases (e. g. α is small) isotropic approximation presents some obvious deviation.

B. Comparison between exact and approximate mode in computing Debye–Waller factor.

To ensure that Fourier transforms are covergent, we have to separate the term which corresponds to zero–phonon scattering. Debye–Waller factor is a coefficient of the separate term.

In fact, if the separate term is just a certain constant, then the Fourier transforms are covergent. If the separate term is not correctly equal to the constant, they may not coverage well. In our code SCAT–3 Debye–Waller factor is calculated by Eq. (26) which is based on exact mode, so Fourier transforms are covergent. If we try to use some approximate mode, for example, to take the following approximation

$$D = \frac{1}{3} D_{//} + \frac{2}{3} D_{\perp} \tag{33}$$

The results as presented in Fig. 2 show that when β is bigger (> 0.2), the results are almost the same; but when β is smaller (< 0.06), the results with approximate Eq. (33) are significantly deviate. This indicate that to take the correct value of Debye–Waller factor is very important.

Table 1 Scattering law calculations for graphite with anisotropic vibrations and with isotropic vibrations

	α	0.07	0.10	0.20	0.40	0.60	1.00	2.00	4.00
β	Methods								
	1	4.40	5.58	7.22	7.03	5.56	3.52	1.55	0.66
0.0	2	4.40	5.58	7.22	7.03	5.56	3.52	1.55	0.66
	3	4.40	5.57	7.21	7.01	5.54	3.51	1.55	0.66
	1	4.09	5.15	6.54	6.42	5.11	3.22	1.44	0.63
0.1776	2	4.08	5.15	6.54	6.41	5.12	3.21	1.43	0.63
	3	3.82	4.85	6.31	5.96	4.62	3.14	1.43	0.63
	1	2.18	2.80	4.07	4.59	4.22	2.84	1.39	0.61
0.2959	2	2.17	2.79	4.06	4.58	4.21	2.83	1.39	0.61
	3	2.04	2.62	3.72	4.18	3.75	2.74	1.39	0.61
	1	0.93	1.23	2.06	2.98	2.97	2.30	1.33	0.59
0.5327	2	0.92	1.23	2.06	2.98	2.97	2.30	1.33	0.59
	3	1.01	1.32	2.09	3.01	2.80	2.32	1.33	0.59
	1	0.52	0.72	1.25	2.01	2.26	2.02	1.27	0.58
0.7694	2	0.52	0.71	1.24	1.99	2.26	2.02	1.27	0.58
	3	0.57	0.79	1.32	2.08	2.28	2.05	1.28	0.58
	1	0.31	0.43	0.82	1.42	1.72	1.73	1.14	0.55
1.0062	2	0.30	0.42	0.81	1.41	1.72	1.73	1.14	0.55
	3	0.32	0.48	0.88	1.51	1.78	1.74	1.14	0.55
	1	0.16	0.25	0.49	0.87	1.16	1.03	0.96	0.51
1.4098	2	0.16	0.24	0.49	0.87	1.16	1.03	0.96	0.51
	3	0.18	0.26	0.52	0.93	1.19	1.03	0.96	0.52
	1	0.082	0.121	0.262	0.492	0.670	0.930	0.780	0.450
1.8979	2	0.082	0.121	0.261	0.492	0.680	0.930	0.780	0.450
	3	0.072	0.110	0.252	0.518	0.740	0.950	0.790	0.451
	1	0.012	0.021	0.069	0.192	0.322	0.507	0.582	0.378
2.4806	2	0.012	0.021	0.069	0.191	0.312	0.506	0.581	0.377
	3	0.010	0.018	0.061	0.177	0.302	0.498	0.580	0.375
	1	0.003	0.007	0.027	0.110	0.246	0.595	0.148	0.205
4.2174	2	0.003	0.007	0.027	0.110	0.246	0.595	0.147	0.205
	3	0.003	0.006	0.023	0.096	0.231	0.593	0.145	0.205

Method 1. GASKET (isotropic)

Method 2. Isotropic mode (in our code SCAT−3)

Method 3. Anisotropic mode (in our code SCAT−3)

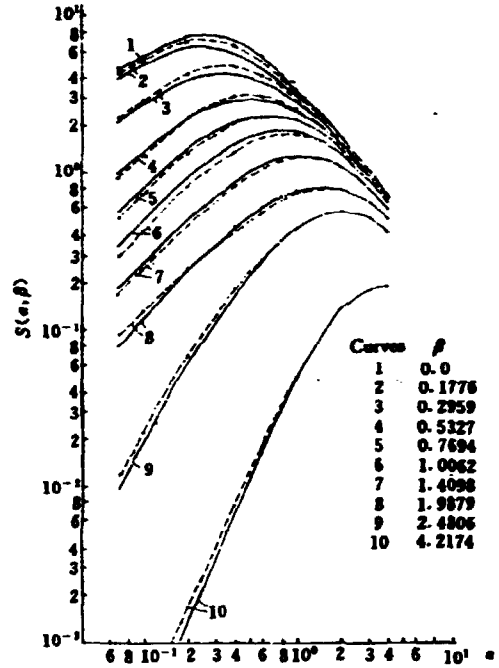

Fig. 1 Scattering law of graphite with anisotropic vibrations (1000 ° K)

---- anisotropic vibrations (combination of modes 1 and 4)

• • • isotropic vibrations (combination of modes 1 and 3)

• GASKET (isotropic vibrations)

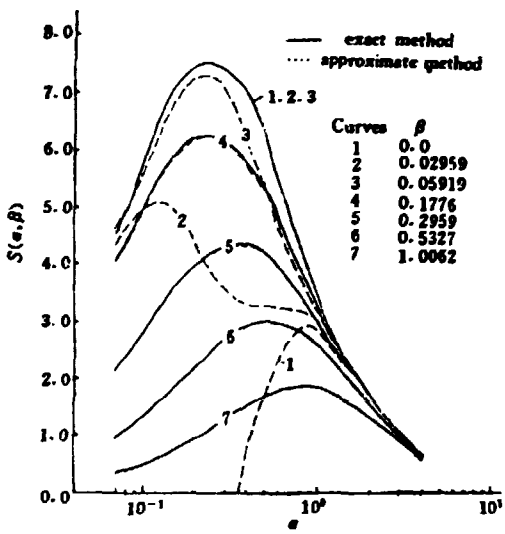

Fig 2 Scattering law with different methods

---- exact method

• • • approximate method

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VII NUCLEAR DATA NEWS

ACTIVITIES AND COOPERATIONS ON NUCLEAR DATA IN CHINA DURING 1992

Zhao Zhixiang

(CHINESE NUCLEAR DATA CENTER, IAE)

1 THE FOLLOWING MEETINGS WERE HELD BY CNDC IN 1992 :

" The 2nd Examination and Acceptance Meeting for Codes Related to Nuclear Data Evaluation " , Apr. 13~ 17, 1992, Gezhouba Electric Power College,Hubei In this meeting, 21 codes related to nuclear model calculation, nuclear data processing, plotting were accepted by Computer Program Library in CNDC.

" The 3rd Working Meeting on Nuclear Structure and Decay Data and 3rd Working Meeting on Data of Charged Particle Induced Reaction ", June 8~ 10,1992, Sichuan University, Chengdu. Reviewed the progress in measurement, calculation and evaluation of nuclear structure and decay data and charged particle induced reaction data.

" The 1st Working Meeting on Chinese Evaluated Nuclear Parameter Library (CENPL)", Nov. 26~29, 1992, Nankai University, Tianjin. Communicated and reviewed the progress in CENPL, discussed some technical problem and arranged the future work.

" Nuclear Data Evaluation Working Group Meeting ", Dec. 2~ 3, 1992, Nankai University,Tianjin. Communicated the progress in data evaluation, discussed some technical problems in evaluation and arranged the future work.

2 THE FOLLOWING INTERNATIONAL CONFERENCES IN DATA FIELD WERE HELD IN CHINA DURING 1992:

" Data Source Task Group Meeting ", Oct. 16~17, 1992, Beijing

" The 13th International CODATA Conference ", Oct. 19~22, 1992, Beij-

ing. 255 scientists, 131 from abroad and 124 from China, attended the conference.

3 THE FOLLOWING INTERNATIONAL MEETING, WORKSHOP ON NUCLEAR DATA FIELD WERE ATTENDED BY CHINESE SCIENTISTS IN 1992 :

" Workshop on Computation and Analysis of Nuclear Data Relevant to Nuclear Energy and Safety ", Feb. 5 ~ Mar. 23, 1992, ICTP, Trieste, Italy.

" NEANSC Specialists' Meeting on Fission Product Nuclear Data ", May 25~27, 1992, JAERI, Japan.

" NEANSC Working Group Meeting on International Evaluation Cooperation ", May 28~29, 1992, JAERI, Japan.

" IAEA Advisory Group Meeting on Technical Aspects of Atomic and Molecular Data Processing and Exchange " , June 15~ 16, 1992, Vienna, Austria.

" The Second Research Co-ordination Meeting on Atomic and Molecular Data for Plasma Edge Studies ", June 17~ 19, 1992, Vienna, Austria.

" IAEA Consultants' Meeting on Technical Aspects of Cooperation of NRDC ", Sep. 1~4, 1992, Vienna, Austria.

" NEANSC Specialists' Meeting on Evaluation and Processing of Covariance Data ", Oct. 7~9, 1992, ORNL, USA.

" IAEA Consultants' Meeting on Charged Particle Nuclear Data and Photon Nuclear Data Libraries for FENDL ", Oct. 8~9, 1992, BNL, USA.

" Symposium on Nuclear Data Evaluation Methodology ", Oct. 12~ 16, 1992, BNL, USA.

" IAEA Advisory Group Meeting on the Network of Nuclear Structure and Decay Data Evaluation ", Dec. 9~13, 1992, Geel, Belgium.

" IAEA CRP Meeting on Calculation of He Production Cross Section ", Dec. 16~18, 1992, Hungry.

4 In 1992, two mumbers of CNDC as visiting scientists worked in ECN / Netherlands and ICTP / Itay in nuclear data field.

5 THE FOLLOWING FOREIGN SCIENTISTS IN NUCLEAR FIELD VISITED CNDC / CIAE IN 1992 AND THE EARLLY OF 1993 :

Three sientists from Dubna in Russia headed by Prof. V. V. Volkov visited

CNDC at Jan. 1, 1992;

Dr. T. Shirai, NDC / JAERI, Japan, Mar. 30 ~ Apr. 1, 1992;

Dr. S. P. Simakov, Obninsk / IPPE, Russia, Apr. 4 ~ 17, 1992;

Dr. T. Narita, NDC / JAERI, Japan, Oct. 11 ~ Dec. 11, 1992;

Dr. T. Fukahori, NDC / JAERI, Japan, Oct. 18 ~ Dec. 11, 1992;

Dr. Y. Kikuchi, NDC / JAERI, Japan, Feb. 20 ~ Mar. 7, 1993.

CINDA INDEX

Nuclide	Quantity	Energy (eV)		Lab	Type	Documentation			
		Min	Max			Ref	Vol	Page	Date
T	Diff Elastic	1.0+3	2.0+7	FUD	Theo	Jour CNDP	9	8	Jun 93
^{7}Li	Evaluation	1.0-5	2.0+7	AEP	Eval	Jour CNDP	9	43	Jun 93
Al	Diff Elastic	1.47+7		TSI	Expt	Jour CNDP	9	1	Jun 93
Ti	(p,γ)	5.1+6	4.4+7	SIU	Eval	Jour CNDP	9	55	Jun 93
Cr	Diff Elastic	1.47+7		TSI	Expt	Jour CNDP	9	1	Jun 93
^{50}Cr	(d,n)	2.0+6	1.2+7	SIU	Eval	Jour CNDP	9	55	Jun 93
^{52}Cr	(p,2n)	2.2+7	4.0+8	SIU	Eval	Jour CNDP	9	55	Jun 93
^{53}Cr	(p,2n)	2.2+7	4.0+8	SIU	Eval	Jour CNDP	9	55	Jun 93
^{55}Mn	(x,2n)	1.3+7	7.9+8	SIU	Eval	Jour CNDP	9	55	Jun 93
	(p,np)	2.2+7	1.5+8	SIU	Eval	Jour CNDP	9	55	Jun 93
Fe	Diff Elastic	1.47+7		TSI	Expt	Jour CNDP	9	1	Jun 93
^{54}Fe	(d,n)	5.0+6	4.0+7	SIU	Eval	Jour CNDP	9	55	Jun 93
^{56}Fe	(p,2n)	1.5+7	3.9+7	SIU	Eval	Jour CNDP	9	55	Jun 93
^{57}Fe	(d,n)	5.0+6	4.0+7	SIU	Eval	Jour CNDP	9	55	Jun 93
Ni	(p,x)	1.1+7	9.8+7	SIU	Eval	Jour CNDP	9	55	Jun 93
Ni	Diff Elastic	1.47+7		TSI	Expt	Jour CNDP	9	1	Jun 93
Mo	(p,x)	2.4+6	1.3+7	SIU	Eval	Jour CNDP	9	55	Jun 93
Pb	Diff Elastic	1.47+7		TSI	Expt	Jour CNDP	9	1	Jun 93
^{238}U	Diff Elastic	1.47+7		TSI	Expt	Jour CNDP	9	1	Jun 93
^{238}U	Evaluation	1.0-5	2.0+7	BJG	Eval	Jour CNDP	9	53	Jun 93

Author, Comments
Wang Yanan+, PHASE SHIFT, ANGDIS
Yu Baosheng+, FOR CENDL-2
Qi Huiquan+, PASS D, ANGDIS
Peng Xiufeng+, SIG
Qi Huiquan+, PASS D, ANGDIS
Peng Xiufeng+, SIG
Peng Xiufeng+, SIG
Peng Xiufeng+, SIG
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Peng Xiufeng+, SIG
Qi Huiquan+, PASS D, ANGDIS
Qi Huiquan+, PASS D, ANGDIS
Tang Guoyou+, FOR CENDL-2

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