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Progress on CENDL-3

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CENDL-3 was started in 1996. Since then, much effort has been made to develop it at CNDC(Chinese Nuclear Data Center) and CNDN(Chinese Nuclear Data Network).

The main progress in 1998 is summarized as following.

1. General Purpose File

According to the plan, CENDL-3 will be completed by 2000, and will contain 200 nuclides. Among them, the data of following nuclides will be newly or reevaluated: fissile nuclides 15, structure materials 18, light nuclides 5, fission products 91. It will contain consistent data between natural elements and their isotopes for structure material, newly evaluated data for fission products, much improved secondary neutron spectra for light nuclides and more r-production data(files 12-15), double differential cross section(file 6).

1) Fissile Nuclides

The evaluation of ^{238}U complete data was completed at Peking University based on the available new experimental data and theory calculation by using codes APOM(automatically adjusting parameter optical model program), FMT(Hauser-Feshbach theory, exiton model), DWUCK and coupled channel optical model. The cross section of inelastic scattering was evaluated and calculated by using coupled channel optical code for first two levels and DWUCK for other higher levels, the result(Fig.1) is consistent with the newly measured data. The neutron double differential cross sections(file 6) were calculated and good agreement(Fig.2) with the data measured by M.Baba and Shen was got by adjusting the parameters of FMT and DWUCK based on above experimental data.

The theoretical calculations have been completed for ^{239}Pu and the evaluation is under way. The results have been compared with the data from ENDF/B-6 and JENDL-3.2. The calculation and experimental data collecting are in progress for other Uranium and Plutonium isotopes.

2) Structure Material

The evaluation of complete data for natural Ni and its isotopes $^{58,60,61,62}Ni$ have been completed and improved. Due to the new experimental data are available in last years, the evaluated data have been considerably improved, especially the (n,p), (n,n'p), (n,α), (n,d), and inelastic scattering cross sections. An example is given in Fig.3. The cross sections between natural Ni and its isotopes are consistent with each other, which was achieved by adjusting them with code CABEI. The energy balance was tested and the energy taken by outgoing particles and the available from the reaction are in balance within several percent.

Also the complete data have been completed for ^{63}Cu, and primary completed for ^{65}Cu. For natural Zr and its isotopes $^{90,91,92,94,96}Zr$, the experimental data have been evaluated and the calculations are under way. For natural Fe and its isotopes $^{54,56,57,58}Fe$, the calculations have been improved and the evaluations of the experimental data are in progress.

3) Light Nuclides

A new model for neutron induced reaction on light nucleus and corresponding code LUNF were developed. The key point of the model is the description of the particle emissions from discrete level to discrete levels in pre-equilibrium states. In the whole reaction processes the angular momentum and parity are conserved and the energy balance is taken into account. The level broadening effect and energy resolution are considered to fit experimental data. Using the code, the calculations for ^{12}C have been completed, and some results are given in Figs.4,5 for total and double differential cross sections respectively. The calculations for other light nuclei are under way.

4) Fission Product Nuclides

According to the plan, the files 1-5 will be included in CENDL-3 for 91 fission product nuclides. So far the evaluations have been completed for 29 nuclides, including theoretical calculation, experimental data evaluation, comprehensive adjusting and checking. The theoretical calculations have been completed for more than 80 nuclides.

2. Special Purpose File

According to the plan, also the special files for fission yield, activation cross section and photonuclear reaction data are being developed.

1) Fission Yield

The reference fission yield were continuously evaluated. The evaluations have been completed in last year for 15 product nuclides of ^{235}U fission and 25 nuclides of ^{238}U fission. They are:

^{235}U fission: ^{85}As, $^{88,89,90,91}Br$, ^{92}Sr, ^{97}Mo, $^{115g,115m}Cd$, ^{135}Sb, $^{135,137}I$, ^{136}Cs, $^{147,152}Sm$;

^{238}U fission: $^{88,89}Br$, $^{85g,85m,87,88}Kr$, ^{91g}Y, ^{95}Zr, ^{99}Mo, ^{106}Ru, ^{105g}Rh, ^{111g}Ag, ^{115m}Cd, ^{125}Sb, $^{131,137}I$, $^{133g,134g}Xe$, ^{140}Ba, ^{144}Ce, $^{147,148}Nd$, ^{151}Sm, ^{156}Eu, ^{161}Tb.

Taking into account of the special features of the retrieval and processing for fission yield data, a fission yield data evaluation system FYDES have been developed. The system includes data retrieval, data table standardization, data correction and data processing(average with weight, simultaneous evaluation and curve fitting etc.). The system has been used for above reference and other yield data evaluations.

2) Activation cross section

The activation cross sections were continuously evaluated for about

40 reaction channels to supplement and improve Chinese Evaluated Nuclear Data File CENDL-ACF. The evaluations were combined with experimental measurements closely, and the recommended data were determined with new measured data at CIAE or other laboratories in China, when the discrepancies were faced in the evaluations. Some examples are given in Figs.6,7. for ^{176}Hf(n,2n) ^{175}Hf and ^{175}Lu(n,2n) $^{174m+g}$Lu respectively.

3) Photonuclear reaction data

The complete data of photonuclear reaction up to 30 MeV, including cross section, double differential cross section, gamma production data of all possible reactions, have been continuously evaluated and calculated by using code GUNF as the task of IAEA CRP. In last year, the evaluations have been completed for nuclides ^{54,56}Fe, ^{209}Bi, ^{63,65}Cu. The evaluations are in progress for nuclides ^{27}Al, ^{9}Be and Cr.

3. Validation of CENDL-2.1

CENDL-2.1 was tested in 1996,1997 for ten homogeneous, eight heterogeneous thermal and nine homogeneous fast assemblies, which were recommended by CSEWG of America. The results show that the calculated Keff in good agreement with experimental ones for U fast, thermal(homogeneous and heterogeneous) assemblies, but they are overestimated for Pu thermal, fast assemblies. This means that the data of ^{235}U, ^{238}U (and O,H) in CENDL-2.1 are reliable, but the data of Pu need to be improved. The similar conclusion also obtained from analysing the calculated reaction rate ratio data for above assemblies.

The benchmark test of CENDL-2.1 was further done in 1998 at NDS by Chinese scientist as visitor guided by Dr. D.Muir. By using Monte Carlo program MCNP-4B, the Keff were calculated for fast assemblies GODIVA, JEZEBEL, and neutron leakage spectra from a fusion neutron source were calculated for many slabs of different materials, such as beryllium, iron, lithium-oxide, oxygen etc. By using code VIMS-D/5A, the integral parameters were calculated for thermal assemblies(table 1).

The conclusion is similar as derived above at CNDC, that is the Keff are in good agreement with experimental ones for all assemblies calculated. The ^{235}U, ^{238}U data of CENDL-2.1 look satisfactory for thermal and fast reactor calculation, but underestimate the fission of ^{238}U in the resonance energy region. For fusion calculation, instead of secondary neutron spectra, the double differential cross sections need to be added for ^{9}Be, ^{16}O and $^{6,7}Li$ in CENDL-2.1.

CENDL-2.1 were also tested for tritium production of $^{6,7}Li$. The tritium production rates were calculated with Monte-Carlo method for theexperiments made by M.E.Wyman, A.Hemmendinger in USA, and Z.Y.Chen in China. The results(table 2) show that the calculated rates are in reasonable agreement with experiments.

Table 1 Integral parameter comparisons

Assembly	Libraries	K-eff	Rho28	Del25	Del28	Convr
TRX-1	Exp.	1.00000(~0.30)	1.320(~1.6)	0.0987(~1.0)	0.0946(~4.3)	0.797(~1.0)
	B6	0.98853(-1.2)	1.377(+4.3)	0.0977(-1.1)	0.0974(+3.0)	0.808(+1.3)
	C2	0.99717(-0.28)	1.379(+4.5)	0.0974(-1.3)	0.0930(-1.7)	0.800(+0.34)
	J2	0.99153(-0.86)	1.370(+3.8)	0.0982(-0.54)	0.0966(+2.1)	0.809(+1.6)
	J3	0.99242(-0.77)	1.370(+3.8)	0.0972(-1.5)	0.0944(-0.18)	0.807(+1.2)
TRX-2	Exp.	1.00000(~0.10)	0.837(~1.9)	0.0614(~1.3)	0.0693(~5.1)	0.647(~0.93)
	B6	0.99113(-0.90)	0.863(+3.1)	0.0600(-2.4)	0.0690(-0.42)	0.650(+0.49)
	C2	0.99842(-0.16)	0.866(+3.5)	0.0599(-2.4)	0.0667(-3.7)	0.0644(-0.43)
	J2	0.99256(-0.75)	0.860(+2.7)	0.0603(-1.7)	0.0688(-0.79)	0.653(+0.87)
	J3	0.99474(-0.53)	0.860(+2.7)	0.0598(-2.6)	0.0674(-2.8)	0.650(+0.46)
BAPL-1	Exp.	1.00000(~0.10)	1.390(~0.72)	0.0840(~2.4)	0.0780(~5.1)	
	B6	0.99431(-0.57)	1.429(+2.8)	0.0824(1.9)	0.0751(-3.7)	0.819
	C2	1.00205(+0.20)	1.435(+3.3)	0.0823(-2.1)	0.0714(-8.5)	0.812
	J2	0.99730(-0.27)	1.421(+2.2)	0.0827(-1.5)	0.0748(-4.1)	0.821
	J2	0.99880(-0.12)	1.422(+2.3)	0.0822(-2.1)	0.0734(-5.9)	0.81
BAPL-2	Exp.	1.00000(~0.10)	1.120(~0.89)	0.0680(~1.5)	0.0700(~5.7)	
	B6	0.99459(-0.54)	1.188(+6.1)	0.0672(-1.2)	0.0645(-7.8)	0.746
	C2	1.00215(+0.21)	1.195(+6.7)	0.0671(-1.3)	0.0617(-12)	0.740
	J2	0.99710(-0.29)	1.183(+5.6)	0.0675(-0.69)	0.0644(-8.0)	0.748
	J3	0.99893(-0.11)	1.183(+5.6)	0.0671(-1.3)	0.0632(-9.7)	0.745
BAPL-3	Exp.	1.00000(~1.0)	0.906(~1.1)	0.0520(~1.9)	0.0570(~5.3)	
	B6	0.99565(-0.44)	0.933(+3.0)	0.0516(-0.67)	0.0528(-7.3)	0.666
	C2	1.00235(+0.23)	0.939(+3.6)	0.0516(-0.67)	0.0509(-11)	0.661
	J2	0.99744(-0.26)	0.929(+2.5)	0.0519(-0.13)	0.0528(-7.4)	0.668
	J3	0.99966(-0.03)	0.929(+2.6)	0.0516(-0.75)	0.0519(-9.0)	0.665
DIMP1A	Exp.	1.00000(~0.10)			0.0962(~3.3)	0.647(~0.46)
	B6	0.99265(-0.74)	4.045	0.2341	0.0862(-10)	0.658(+1.7)
	C2	1.00246(+0.24)	4.060	0.2340	0.0836(-13)	0.653(+0.90)
	J2	0.99782(-0.22)	4.025	0.2351	0.0852(-11)	0.658(+1.7)
	J3	0.99989(-0.01)	4.019	0.2328	0.0836(-13)	0.656(+1.4)
Average	Exp.	(0.15)	(1.32)	(1.69)	(4.86)	(0.83)
	B6	-0.73(~0.25)	3.85(~1.25)	-1.44(~0.62)	-4.45(~4.60)	1.16(~0.49)
	C2	0.08(~0.21)	4.30(~1.26)	-1.54(~0.63)	-8.27(~4.19)	0.27(~0.54)
	J2	-0.44(~0.26)	3.38(~1.22)	-0.92(~0.60)	-4.94(~4.57)	1.36(0.35)
	J3	-0.26(~0.28)	3.40(~1.23)	-1.66(~0.65)	-6.78(~4.35)	1.02(0.40)

Note : The meaning of the abbreviation in the Table 8 is as following

Rho28 — epithermal / thermal capture for ^{238}U

Del25 — epithermal / thermal fission for ^{235}U

Del28 — ^{238}U / ^{235}U fission

Convr — ^{238}U capture/ ^{235}U fission

Table 2 The comparison between the calculations and the experiments

Laboratory	reaction ratios	experiments	ENDF/B-6	CENDL-2.1
Chen (China)	P_T^6	0.79±0.07(*) 0.75±0.04(**)	0.7614	0.7708
Hemmendinger (USA)	P_T^6	0.853	0.7913(#) 0.8163(##)	0.7984(#) 0.8234(##)
Wyman (USA)	P_T^7	0.43±0.004	0.4196	0.4200

where : * measured by the proportional counter ; # not including P_T^7 ;

** measured by the scintillation detector ; ## including P_T^7 ;

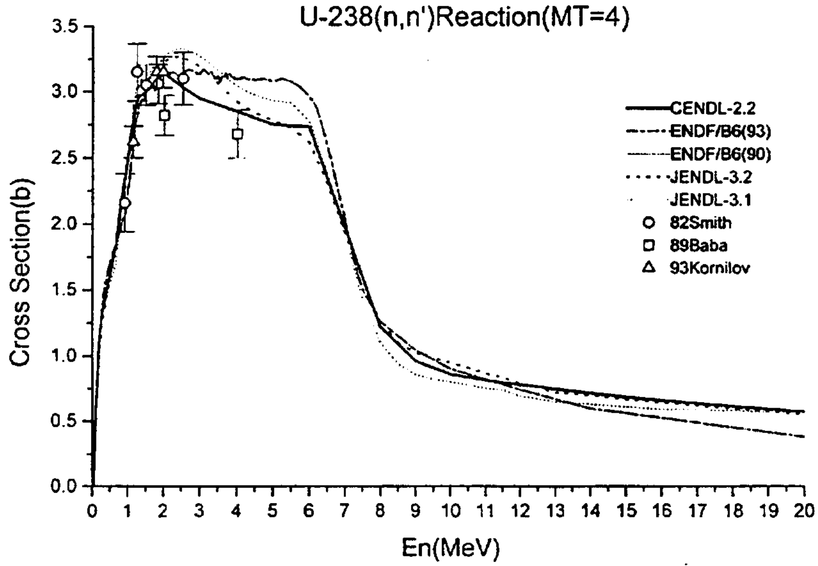

Fig.1 The evaluated cross section of ^{238}U total inelastic cross section

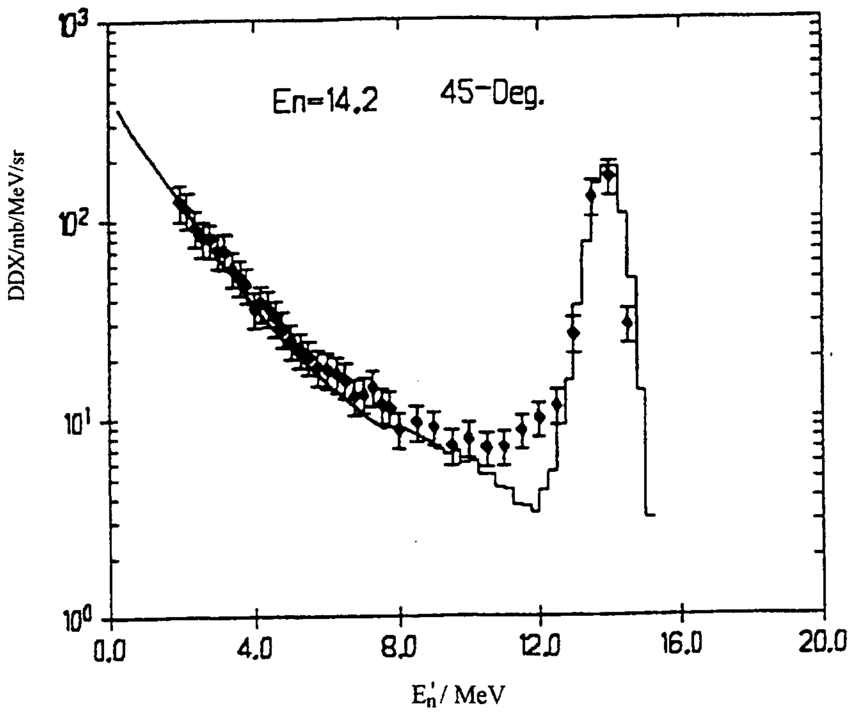

Fig. 2.1 The evaluated double differential cross section of ^{238}U (n, n emission) at E_n=14.2 MeV (θ = 45°)

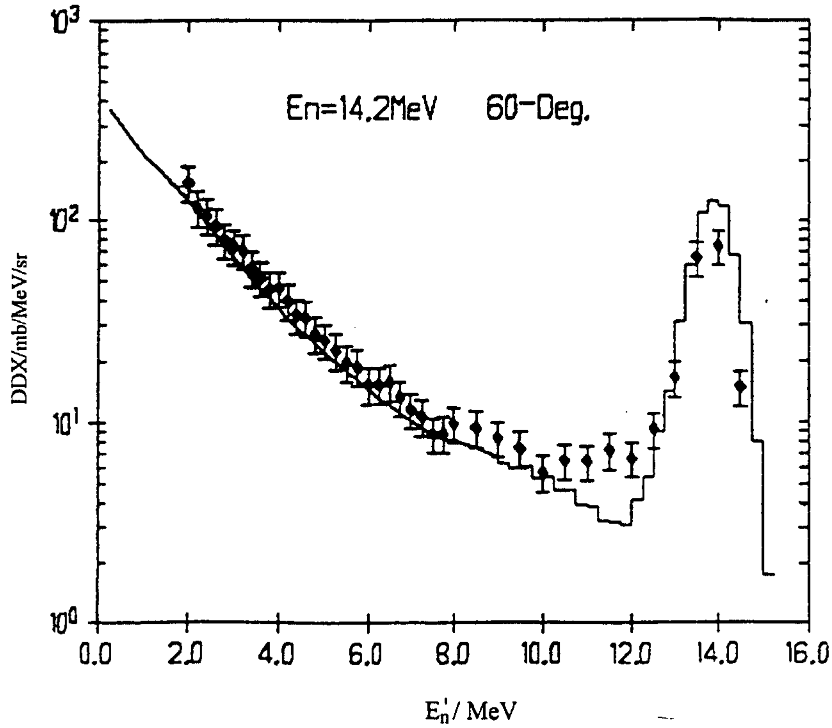

Fig. 2.2 The evaluated double differential cross section of ^{238}U (n, n emission) at E_n=14.2 MeV (θ = 60°)

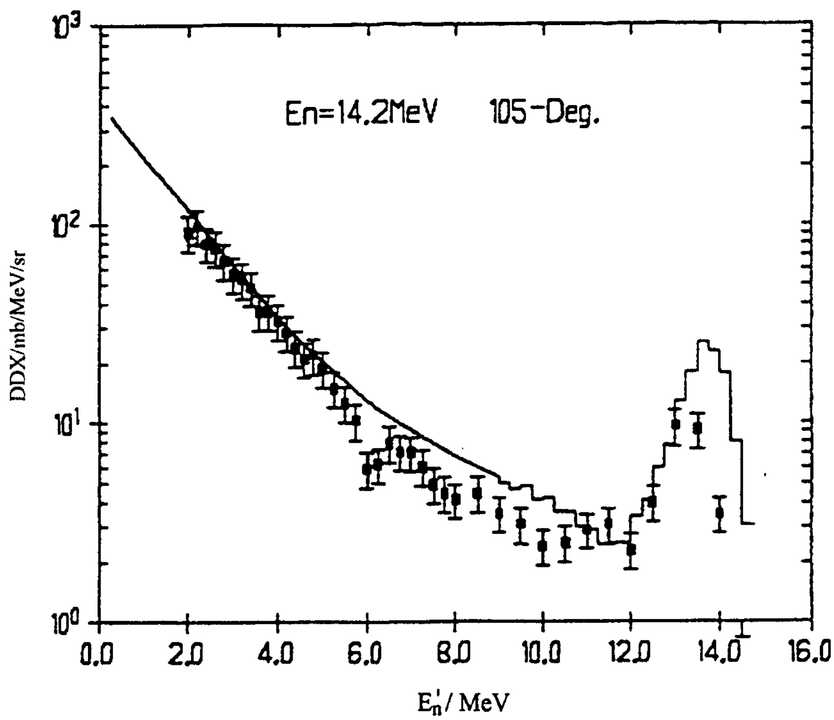

Fig. 2.3 The evaluated double differential cross section of ^{238}U (n, n emission) at E_n=14.2 MeV (θ = 105°)

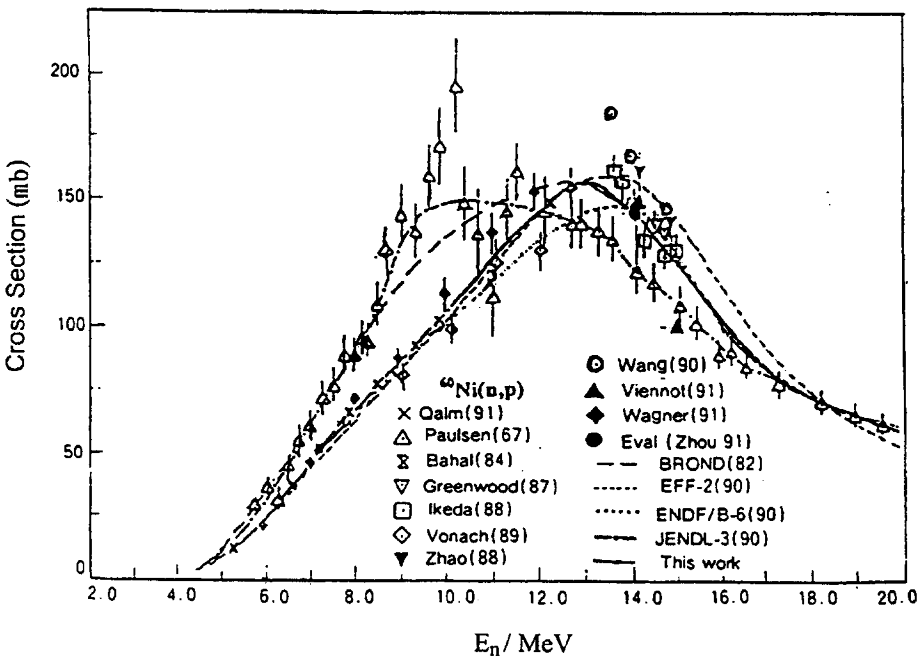

Fig. 3 The calculated total cross section of ^{60}Ni (n, p) reaction

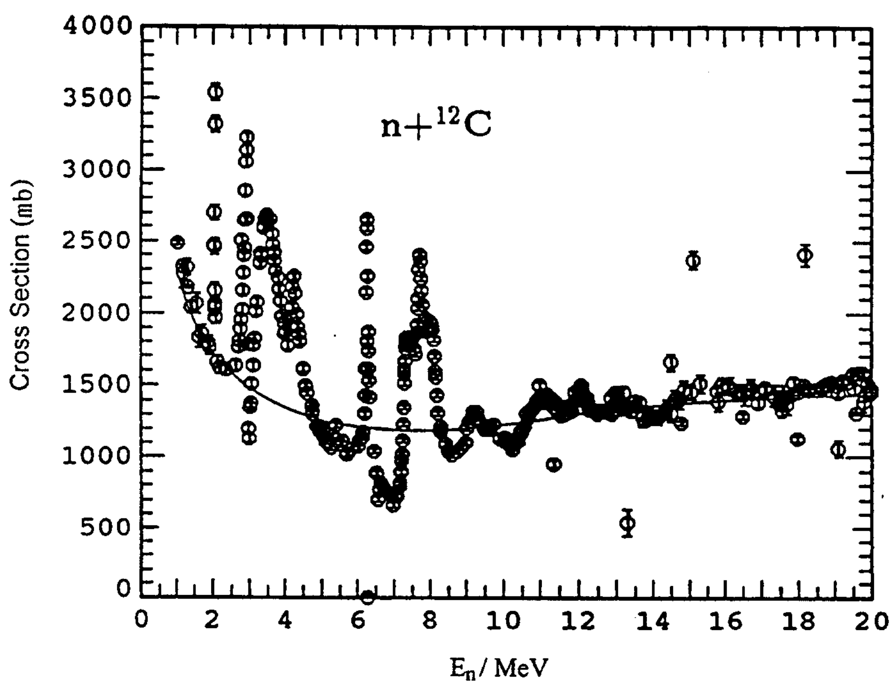

Fig. 4 The calculated total cross section of n + ^{12}C reaction

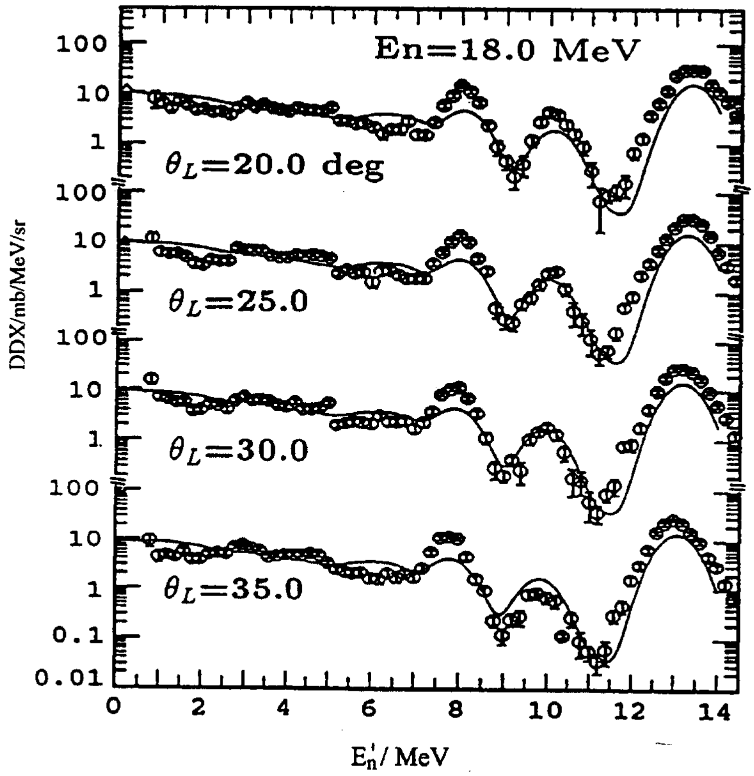

Fig. 5.1 The calculated DDX of [12]C (n, n emission) at En = 18.0 MeV compared with measured data by Baba (1990) (θ =20° - 35°)

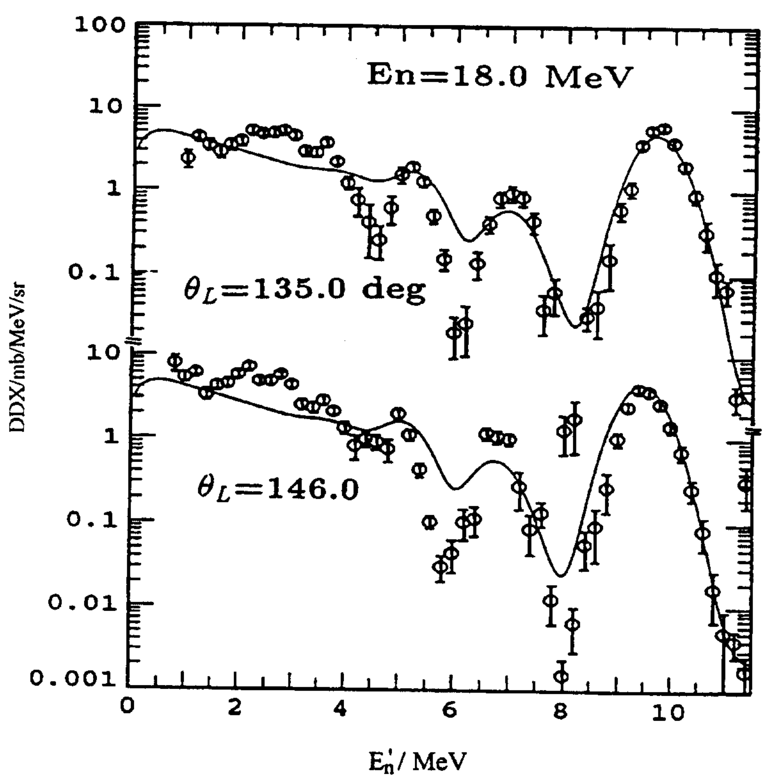

Fig. 5.2 The calculated DDX of [12]C (n, n emission) at En = 18.0 MeV compared with measured data by Baba (1990)(θ =135°- 146°)

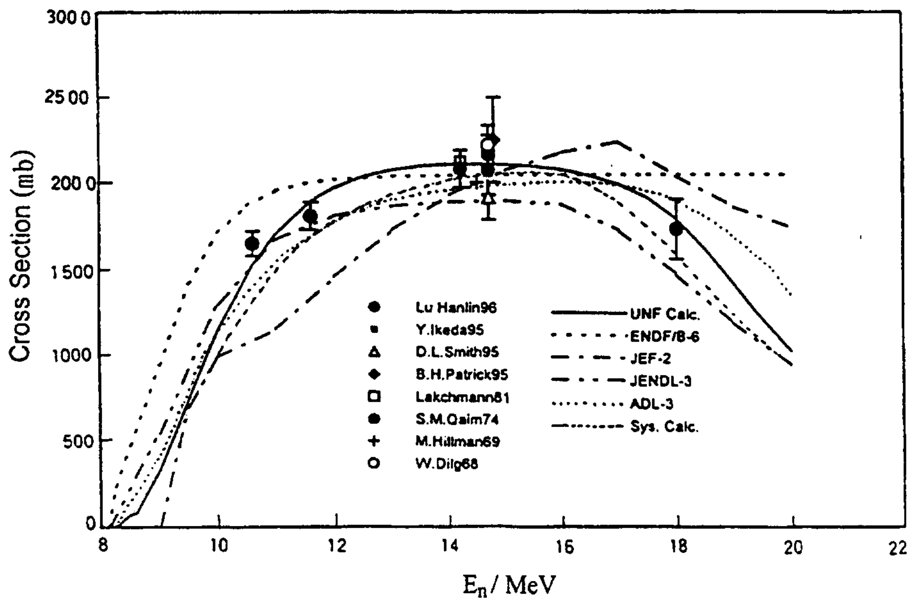

Fig. 6 The evaluated cross section of ^{176}Hf (n, 2n) reaction based on new measured data at CIAE

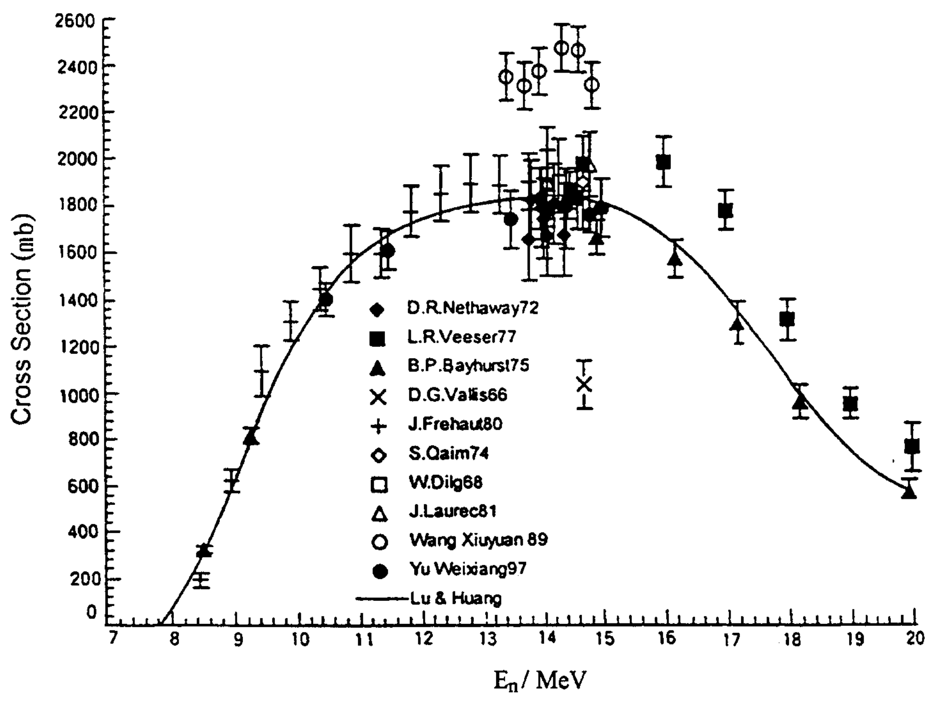

Fig. 7 The evaluated cross section of ^{175}Lu (n, 2n) $^{174m+g}$Lu reaction based on new measured data at CIAE