Beta-delayed gamma spectra in CENDL-3.2

Shuyu Zhu[1], *Xiaoxue* Zhao[1,2], *Nengchuan* Shu[1*], *Haicheng* Wu[1], *Lin* Liu[2*], *Yongjing* Chen[1], *Lile* Liu[1]

[1]China Nuclear Data Centre, 102413, Beijing, China
[2]College of physical science and technology, Shenyang Normal University, 110034, Shenyang, China

Abstract. A new program is developed to compute the beta delayed fission gamma spectrum, and applied to compute the spectra of n+^{235}U, ^{239}Pu and ^{241}Pu fissions wherein the recent nuclear database is adopted. The results show that most spectra are well in agreement with the data from ENDF/B-VII.0 library, and some are quite different, which should be caused by the improvement of the nuclear database.

1 Introduction

The beta delayed fission gamma spectrum (hereafter called BDFG), also named the delayed gamma source function in ENDF formats manual [1], is formed by the emitted gammas during the fission products beta decay, which could be used in such as reactor shielding, spent fuel decay heat and fission experiment simulation etc, and also could check the product fission yields compared to their measured gamma spectra.

BDFG is stored in ENDF-6 format with MT = 460 and MFs=1, 12, 13, standing for the normalization coefficient, normalized spectrum as function of time, and angular distribution, respectively. There are only 2 sets of BDFG of n+^{235}U and ^{239}Pu fission in ENDF/B-VII.1 library, which should be contributed in 2004 or so [2].

The motivation of this work is to develop a different method with Ref. [2] to calculate the BDFG of n+^{235}U and ^{241}Pu, make update and supplement for the BDFG library with new nuclear database.

2 Calculation Method

The beta delayed fission gamma spectrum, is defined as the gamma number emitted per unit time per unit gamma energy after a certain fission event [1],

$$S_\gamma(t, E_\gamma) \equiv \frac{d^2 n}{dE_\gamma dt}(t, E_\gamma). \quad (1)$$

And it could be calculated as the following formula,

$$S_\gamma(t, E_\gamma) = \int_t^{t+1} \sum_{i,j} \delta(E - E_\gamma) \lambda_i n_i(t) I_{i,j}(E_\gamma)\, dt, \quad (2)$$

where t is the time following fission at which the gamma is emitted, E_γ the emitted gamma energy, λ_i the decay constant of nuclide i, $I_{i,j}$ the intense of j^{th} gamma of the nuclide i, n_i is the abundance of nuclei i, which is a function time t, could be calcuated by resloving the ordinary differential equations,

$$\frac{dn_i(t)}{dt} = -\lambda_i n_i(t) + \sum_j \lambda_{j\to i} n_j(t), \quad (3)$$

$$n_i(0) = y_i \quad (4)$$

where the first item on the left of eq. (3) is nuclide i decaying to others, and the second item is the precursor nuclide j decay into this i nuclide. This equation could be calculated with burn-up codes such as CINDER [3] or Origen[4]. The inital numbers at t=0 are given with the independent yields in eq. (4).

In this work, a gamma summation code named FP.pl (Fission Photon) is created. It reads the number $n_i(t)$ of fission products from the calculation result of eqn (3) and (4), compute the individual spectrum as a function of time t for each gamma emitted. And then make the summation of all the individual spectra to produce the total BDFG, $S\gamma$. Fission yields are taken from ENDF/B-VII.1 and decay data from NuDat (2017) [5].

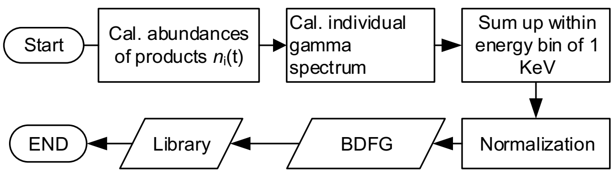


Fig. 1. The main flow of FP.pl code.

Given the parameters of a fission experiment, gamma counts could be simulated based upon the BDFG, S_γ as

$$N_\gamma(E_\gamma, \ t_c \to t_c + t_d) = f(E_\gamma) \int_{t_c}^{t_c+t_d} \int_0^{t_r} f_r(t_r) S_\gamma(t + t_r, E_\gamma)\, dt_r\, dt, \quad (5)$$

where t_c, t_d are the cooling and detecting times resp., $f(E_\gamma)$ the factor including detector efficience, dead time corretion, gamma absorb correction, geometric correction, conversion of calcualted count to measured count etc. t_r the radiating time of sample, and $f_r(t_r)$ is the fission rate function, these paramters are provided by the exprimenter.

Corresponding author: nshu@ciae.ac.cn

To verify the code FP.pl, BDFGs of n+^{235}U are calculated and compared with those in ENDF/B-VII.1. They agree very well at most energies such as shown in Fig.2 and Fig.3, but some do not, as shown in Fig. 4 which should be caused by the improvement of the new nuclear data base in this work.

Simulation of a fission experiment is performed with eq. (5), the result is illustrated in Fig. 5, the calculated gamma counts are in good agreement with measured counts, where '138Cs' at 1009.8 keV should be combined with the gamma at 1010 keV emitted from ^{142}La. This experiment was carried out in China Nuclear Data Centre.

The above comparisons verified the FP.pl code, and showed the present results are improved with new nuclear database.

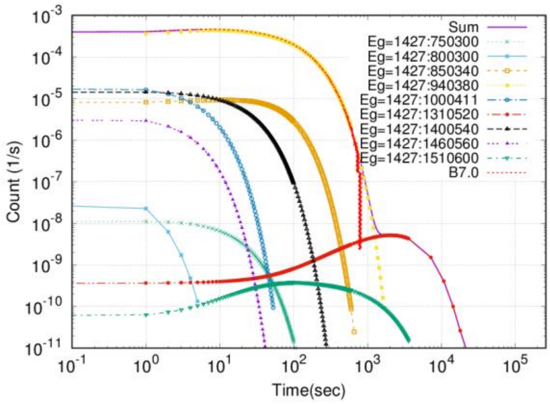


Fig. 2. Calculated BDFGs at E_γ=1427 keV, compared with that in ENDF/B-VII.0 for n_{th}+^{235}U fission. The legend such as '1427:750300' denotes the γ (1427KeV) emitted from the decay of nuclide A*1000+Z*100+Isomer (A=75, Z=30, Isomer=0)

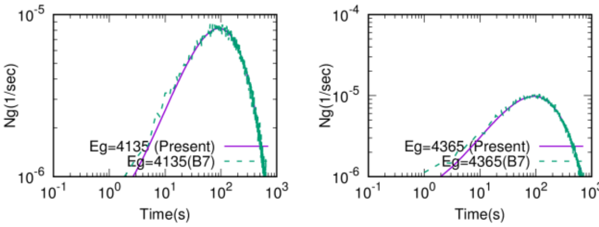


Fig. 3 Calculated BDFGs at E_γ=4135 and 4365 keV compared with those in ENDF/B-VII.1 for n_{th}+^{235}U fission.

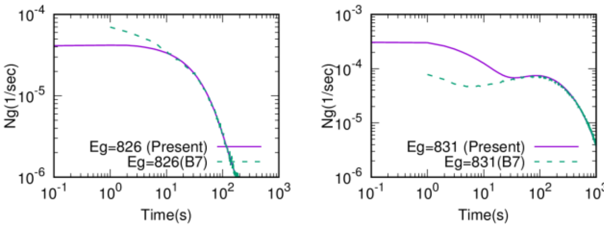


Fig. 4 Calculated BDFGs at E_γ=826 and 831 keV compared with those in ENDF/B-VII.1 for n_{th}+^{235}U fission.

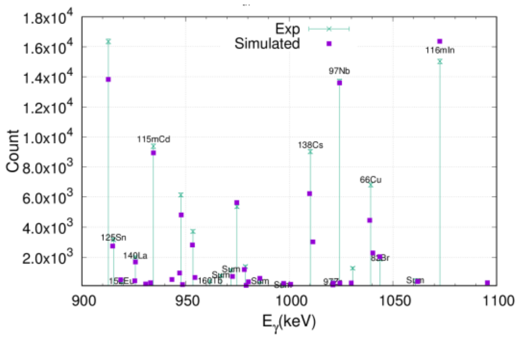
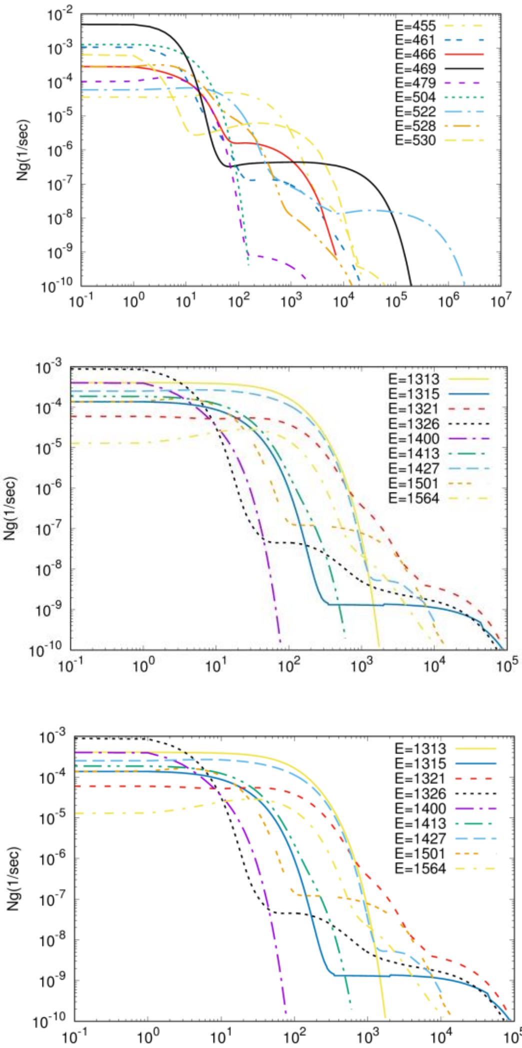


Fig. 5. Simulated gamma counts compared with the measured.

3 BDFG calculation of n+^{241}Pu fission

The beta delayed fission gamma spectra of n+^{241}Pu are calculated with incident neutron of thermal and fission spectrum. Part of the results of n_{th}+^{241}Pu are shown in Fig.6, which counts (coefficients) are larger than 0.001 at variant energy regions around 500, 1000, 1500 and 2000 keV. There are about 50 coefficients are large than 0.01 and listed in Table. 1.



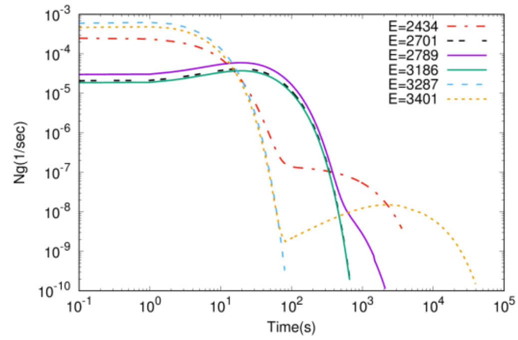


Fig. 6. The BDFG of n_{th}+^{241}Pu fission at variant energies as functions of the decay time.

The integrals of BDFG are calculated over the gamma energy regions of 0-6950, 1000-2000, 2000-3000, 3000-4000, 4000-6950 keV. As shown in Fig.7, the total gamma count rate at zero time is about 0.2 per second, this hints that there is 0.02 beta delayed gamma emitted in the first second after one fission. The others are about 0.03, 0.002 and 0.0002 per second (Fig.4), contributing about 15%, 1% and 0.1% to the total. And the BDFG within 0-1000 keV contributes most of the total gammas, about 84%.

The total gamma number decreased rapidly during 1 - 100 seconds, about 10^4 seconds later, it is less than 0.1% of the primary counts at zero time.

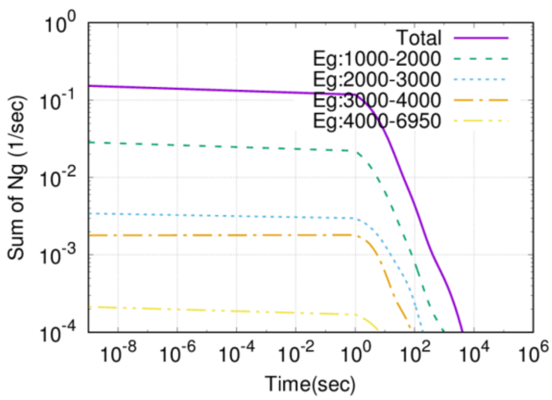


Fig. 7. Integral of BDFG over variant energy regions as functions of the decay time for n_{th}+^{241}Pu fission.

Table 1. BDFG Coefficients (>0.01) of n+^{241}Pu fissions.

Eγ(KeV)	En=T	En=F	T/F
2	1.91E-02	1.96E-02	1.00
13	1.31E-02	1.38E-02	1.10
17	9.22E-02	9.41E-02	1.00
18	7.75E-02	7.94E-02	1.00
19	1.87E-02	1.84E-02	0.98
20	1.44E-02	1.44E-02	1.00
32	1.17E-02	1.22E-02	1.00
33	1.17E-02	1.14E-02	0.97
36	1.63E-02	1.68E-02	1.00
43	1.29E-02	1.34E-02	1.00
68	2.95E-02	2.98E-02	1.00
85	1.44E-02	1.58E-02	1.10
97	1.64E-02	1.52E-02	0.93
119	8.71E-03	1.08E-02	1.20
121	1.64E-02	1.71E-02	1.00
122	1.98E-02	2.19E-02	1.10
137	2.94E-02	2.74E-02	0.93
161	1.12E-02	1.01E-02	0.90
197	1.61E-02	1.42E-02	0.88
211	1.17E-02	1.20E-02	1.00
258	1.37E-02	1.30E-02	0.95
270	2.92E-02	2.97E-02	1.00
276	1.44E-02	1.50E-02	1.00
296	3.34E-02	3.58E-02	1.10
381	1.68E-02	1.42E-02	0.85
397	3.42E-02	3.39E-02	0.99
400	1.12E-02	1.11E-02	0.99
447	9.58E-03	1.03E-02	1.10
469	2.98E-02	2.77E-02	0.93
504	1.60E-02	1.59E-02	0.99
535	2.96E-02	2.82E-02	0.95
541	1.33E-02	1.31E-02	0.98
546	2.58E-02	2.40E-02	0.93
551	1.25E-02	1.34E-02	1.10
588	1.41E-02	1.19E-02	0.84
593	1.52E-02	1.42E-02	0.93
602	2.26E-02	2.09E-02	0.92
603	1.08E-02	1.09E-02	1.00
724	1.13E-02	1.16E-02	1.00
809	1.85E-02	2.06E-02	1.10
1103	1.54E-02	1.40E-02	0.91
1222	1.42E-02	1.22E-02	0.86
1313	3.16E-02	2.85E-02	0.90
1427	2.11E-02	2.10E-02	1.00
1632	1.70E-02	1.82E-02	1.10
1750	1.39E-02	1.10E-02	0.79

4 Build of BDFG library

The beta delayed fission gamma spectra are converted to ENDF/B-VI format as descripted in ENDF-6 format manual which MT is 460, and there are 3 files MF=1, 12 and 13. The general information is described in Table 2 for the case of ^{241}Pu.

MF=1 of MT=460 is the normalized BDFG, as shown in Table 3. The first column data in line 2 and line 11 are the gamma energies in eV (here are 6.95E6 and 6.794E6). Line 4-10 and 13-19 are the two normalized BDFGs with 2 data (time, count) in group, the group numbers are ‘20’ and ‘19’ as indicated in line 3 and 12, respectively.

MF=12 of MT=460 is the normalization coefficients, as shown Table 4. Line 6 indicates the energy in the first column (here is 6.95E6) corresponding to that one in MF=1. Line 8-9 are the 6 groups of the coefficients; each group contains two data of the incident neutron energy in eV and coefficient in 1/sec. MF=14 is the angular distribution. More detail information could be found in the ENDF-6 manual. The database of n+^{235}U, ^{239}Pu and ^{241}Pu BDFGs have been checked and complied into CENDL-3.2, the main text lines are listed in Table 2 for the case of ^{241}Pu.

Table 2. Beta-delayed fission gamma spectrum of n+^{241}Pu fission in ENDF-6 format (MF=1, MT=451, general information)

```
CENDL-3.2                                                            1 0  0    0
 9.424100+4 2.389880+2          1          1          5          39443 1451    1
 0.000000+0 1.000000+0          0          0          0          69443 1451    2
 1.000000+0 2.000000+7          2          0         10          39443 1451    3
 0.000000+0 0.000000+0          0          0        381         749443 1451    4
 94-Pu-241          EVAL-                                         9443 1451    5
                    DIST-                                         9443 1451    6
----CENDL-3         MATERIAL 9443                                 9443 1451    7
-----INCIDENT NEUTRON DATA                                        9443 1451    8
------ENDF-6 FORMAT                                               9443 1451    9
HISTORY                                                           9443 1451   17
2019-05 Delayed gamma data (MT460) were evaluated and compiled by 9443 1451   27
       Nengchuan SHU and Haicheng WU.                             9443 1451   28
*********************** C O N T E N T S *********************** 9443 1451  385
                                1        451        459          29443 1451  386
                                1        460     232740          39443 1451  391
                               12        460      14657          39443 1451  458
                               14        460          1          39443 1451  459
```

Table 3. Main text lines of beta-delayed fission gamma spectrum of n+^{241}Pu fission in ENDF-6 format (MF=1, MT=460, normalized beta-delayed fission gamma spectrum as function of time)

```
9.42390+04 2.36999+02          1          0       3666          09437 1460    1
6.95000+06          0          1          0          1         209437 1460    2
        20          4                                            9437 1460    3
         0 3.79723-01 1.00000+00 2.35728-01 2.00000+00 1.46153-019437 1460    4
3.00000+00 9.06151-02 4.00000+00 5.61817-02 5.00000+00 3.48328-029437 1460    5
6.00000+00 2.15965-02 7.00000+00 1.33900-02 8.00000+00 8.30193-039437 1460    6
9.00000+00 5.14731-03 1.00000+01 3.19146-03 1.10000+01 1.97881-039437 1460    7
1.20000+01 1.22697-03 1.30000+01 7.60825-04 1.40000+01 4.71815-049437 1460    8
1.50000+01 2.92629-04 1.60000+01 1.81533-04 1.70000+01 1.12653-049437 1460    9
1.80000+01 6.99471-05 1.90000+01 4.34697-05                      9437 1460   10
6.79400+06          0          2          0          1         199437 1460   11
        19          4                                            9437 1460   12
         0 3.79740-01 1.00000+00 2.35739-01 2.00000+00 1.46159-019437 1460   13
3.00000+00 9.06190-02 4.00000+00 5.61842-02 5.00000+00 3.48344-029437 1460   14
…
```

Table 4. Main text lines of beta-delayed fission gamma spectrum of n+^{241}Pu fission in ENDF-6 format (MF=12, MT=460, normalization coefficient)

```
9.42390+04 2.36999+02          1          0       3665          0943712460    1
0.000000+0 0.000000+0          0          0          1          6943712460    2
         6          2                                            943712460    3
1.00000-05 2.19709+00 1.00000+05 2.19709+00 1.00000+05 2.19709+00943712460    4
7.00000+06 2.19709+00 7.00000+06 2.19709+00 2.00000+07 2.19709+00943712460    5
6.95000+06 0.00000+00          0          2          1          6943712460    6
         6          2                                            943712460    7
1.00000-05 3.54224-08 1.00000+05 3.54224-08 1.00000+05 3.54224-08943712460    8
…
```

5 Remarks

A new code FP.pl has been created and verified calculate the beta-delayed fission gamma spectrum with recent updated nuclear database. The beta-delayed fission gamma spectrum of n+^{235}U, ^{239}Pu and ^{241}Pu fissions are calculated and complied into CENDL-3.2.

This work was supported by national nature science foundation of China (No. 11790320, 11790323, 11790324, 11790325 , U1867213), the continuous Basic Scientific Research Project (No. WDJC-2019-09)

References

[1] A. Trkov, M. Herman and D. A. Brown, *ENDF-6 Formats Manual*, Report BNL-90365-2009 Rev.1(2010). p.49.

[2] J. Pruet et al., Nucl. Inst. Meth. B 222, 403 (2004).

[3] W. Wilson, S. Cowell, T. England et al. *A Manual for CINDER'90 Version 07.4 Codes and Data* [R]. Los Alamos National Laboratory, LA-UR-07-8412.

[4] G. Croff, *A User's Manual for the ORIGEN2 Computer Code*. ORNL/TM-7175, Oak Ridge National Laboratoly, 1980.

[5] http://www.nndc.bnl.gov