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Development of JENDL FP Decay Data File 2000

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JENDL FP Decay Data File 2000 has been developed as a special purpose file of JENDL. The file contains various decay data of fission product nuclides needed for the analyses of FP accumulation, decay heat, aggregate beta- and gamma-ray spectra and so on in a nuclear reactor. The number of unstable nuclides including isomeric states is 1087.

KEYWORDS: fission product, decay data, average decay energy, beta- and gamma-ray spectra

I. Introduction

Decay data of fission product nuclides are needed for various kinds of nuclear technology fields, such as decay heat, FP accumulation, radiation shielding and so on. Decay Heat Evaluation Working Group, Japanese Nuclear Data Committee has developed a decay data file mainly for decay heat evaluation in a reactor. The group released JNDC Nuclear Data Library for Fission Products, -Second Version- [1](hereafter JNDC-V2), in 1990. The library, however, has a unique format different from the ENDF format[2] which is used in JENDL (Japanese Evaluated Nuclear Data Library). In the course of the plan revising the JNDC-V2 library, the idea to compile a decay data file of fission product nuclides as a JENDL special purpose file came out. Then the JENDL FP Decay Data File 2000[3] (hereafter JENDL-FPDD) has been developed.

The decay data in the JNDC-V2 library have been successfully applied to the decay heat calculation of fissionable nuclides. Then the data in the JNDC-V2 library can be adopted in the JENDL file. The measured data adopted in the JNDC-V2 library, however, are those taken more than 10 years ago and it has become hard to indicate the original data source. Then it was decided to use ENSDF[4] (Evaluated Nuclear Structure Data File) as a data source of the measured data. The decay data in the ENSDF file are based on the measurement and does not cover all of the nuclides needed for the compilation of the JENDL-FPDD file. It is also known that there is a so called "Pandemonium Problem"[5] in the data of some nuclides with high Q values and short half-lives. The problem is that the average decay energy value of beta-ray is enhanced and that of gamma-ray depressed for such nuclide. For the nuclides having the problem the theoretically estimated data in the JNDC-V2 library have been adopted in the JENDL-FPDD file.

As mentioned above the JNDC-V2 library is for decay heat calculation, the spectral data are not included. In the compilation of the JENDL-FPDD file, the spectral data of beta- and gamma-rays are needed. The measured spectral data have been taken from the ENSDF file and those of the nuclides having no or incomplete data have been newly estimated by a theoretical model.

In this report the decay data in the JENDL-FPDD file are briefly described. The decay heat and spectrum calculations using the JENDL-FPDD file are also presented.

II. Characteristic of the Decay Data in the JENDL-FPDD File

The JENDL-FPDD file contains the decay data of 1087 unstable fission product nuclides which covers mass numbers of 66 through 172. As there are 142 stable nuclides in this mass region, total number of FP nuclides in the JENDL-FPDD file amounts to 1229. The decay data contained in the JENDL-FPDD file are half-life, decay modes, their Q values and branching ratios, average decay energy values of radiations and their spectra. They are arranged in the format of ENDF file. In the compilation of the JENDL-FPDD file, the measured decay data are reviewed and adopted from the ENSDF file if they are available.

One of the characteristic of the JENDL-FPDD file is the adoption of theoretically estimated decay data. Of 1087 unstable nuclides in the JENDL-FPDD file, about half of them have the measured decay data. The decay data of the rest have to be estimated by theoretical method or systematics. We have employed a theoretical model called "Gross Theory of Beta Decay".[6] The gross theory expresses the gross properties of beta decay with the aid of sum rule. In this model individual discrete levels are treated as continuous one. In this model, the average beta- and gamma-ray energy values are described as:[7]

$$\begin{aligned}\bar{E}_\beta &= \frac{1}{2\pi^3\lambda}\int_{-Q}^{0}\sum_{\Omega}|g_\Omega|^2\cdot|M_\Omega(E_g)|^2 \\ &\quad\times\int_{1}^{-E_g+1} mc^2(E-1)pE(-E_g+1-E)^2 \\ &\quad\times F(E)dEdE_g,\end{aligned} \tag{1}$$

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$$\bar{E}_\gamma = \frac{1}{2\pi^3\lambda}\int_{-Q}^{0}\sum_{\Omega}|g_\Omega|^2\cdot|M_\Omega(E_g)|^2mc^2(Q+E_g) \times\int_{1}^{-E_g+1} pE(-E_g+1-E)^2F(E)dEdE_g, \quad (2)$$

where

λ = beta decay constant,
F = Fermi function,
p = electron momentum,
m = electron mass,
c = speed of light.

The beta decay constant λ is expressed as:

$$\lambda = \frac{1}{2\pi^3}\int_{-Q}^{0}\sum_{\Omega}|g_\Omega|^2\cdot|M_\Omega(E_g)|^2f(-E_g+1)dE_g, \quad (3)$$

where E_g is the partial decay energy and is related to the excitation energy E_i as $E_g = -(E_i - 1)$. The function $f(-E_g+1)$ is the integrated Fermi function. The notation $\sum_\Omega|g_\Omega|^2\cdot|M_\Omega(E_g)|^2$ is used for the beta-strength function. The symbol of Ω refers to types of the beta transition, Fermi, Gamow-Teller and so on. The essence of the gross theory lies in a way to evaluate the strength function with the aid of sum rules and a relatively simple nuclear model. The beta- and gamma-ray spectra have been also estimated using the strength function.[8,9]

In the case of the spectrum data, the adoption of the theoretical estimation[10] has been performed to keep the measured spectrum. This means that the theoretically estimated spectrum has been used only to compensate the measured spectrum when measured spectrum is available but is considered to be incomplete. So the nuclides with incomplete spectrum data have two kinds of data, that is, measured data and estimated ones. This situation is seen in **Table 1** where the number of various kinds of nuclides is listed. For example 1053 nuclides have gamma-ray spectrum data as seen in this table. Of these nuclides 126 nuclides have both measured and theoretically estimated spectra. Their measured spectra have been considered to be incomplete. And they have been compensated with the theoretical estimation. In the incomplete measured data, only low lying levels of a daughter nucleus are identified although there must be some levels in unobserved energy region. The beta transitions to the unobserved region have been calculated with the gross theory.

Examples of the compensation are shown in **Figs. 1** and **2**. **Figure 1** shows beta ray spectrum of ^{89}Br decay. The Q value of the decay is 8.16 MeV, but the maximum energy of the observed level is much less than the Q value. The levels located between the maximum energy and the Q value may not be observed experimentally even if there is a possibility that some missing levels exist. The beta transitions to the region has been calculated and used to compensate the measured spectrum. The measured spectrum is designated as "Measured" and the calculated one as "Calculated" in the figure. "Compensated" in the figure is constructed by merging them using suitable normalization factors as follows.

$$S_e(E) = \alpha\cdot S_m(E) + \beta\cdot S_c(E), \quad (4)$$

where $S_e(E)$ is the compensated spectrum, $S_m(E)$ the measured one and $S_c(E)$ the calculated one. α and β are the normalization factors. The normalization factors have been determined to give the average decay energy value used for

Table 1 General Contents of the Data in the JENDL-FPDD File

No. of Nuclides		Data Types, Comments
1229		Total number of nuclides
142		Stable nuclides
1087		Unstable nuclides or states
581		With theoretically estimated average gamma decay energy value
506		With measured average gamma decay energy value (including x-ray energy)
543		With theoretically estimated average beta decay energy value
544		With measured average beta decay energy value (including conversion electron energy)
1053		With gamma-ray spectrum data
	431	With theoretically estimated spectrum only
	496	With measured spectrum only
	126	With measured and theoretically estimated spectrum
899		With beta-ray spectrum
	432	With theoretically estimated spectrum only
	374	With measured spectrum only
	93	With measured and theoretically estimated spectrum

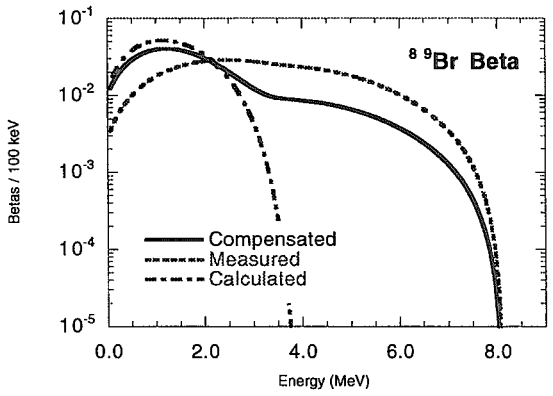

Fig. 1 Compensation of beta ray spectrum

decay heat analysis when the integration of the spectrum for whole energy region is performed. By this way the consistent calculations of decay heat and spectrum are able to be carried out.

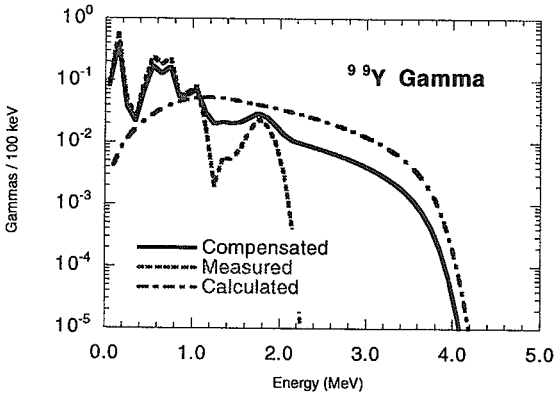

Fig. 2 Compensation of gamma ray spectrum

Figure 2 shows gamma ray spectrum of ^{99}Y decay. In the case of the gamma ray spectrum, the beta transitions to the region of unobserved levels calculated with the gross theory and the cascade transition model of gamma transition have been used. The calculated gamma ray spectrum is given as a continuous spectrum though actual gamma ray spectrum is a discrete one. This situation is seen in **Fig. 2**. The measured spectrum designated as dotted line has the structure which is due to the line character of the spectrum but is broadened arbitrary in this case for easy seeing. The discrete measured spectrum and the continuous calculated spectrum have been merged into "Compensated" spectrum using the equation 4 like the beta ray spectrum.

III. Decay Heat Calculation

Decay heat of fission products produced after fission of a fissionable nuclide has been calculated and compared with measured data. The decay heat is usually represented by energy release rate due to the decay of radioactive nuclides generated by fission event. The decay heat of fission product nuclides at t s after a fission burst, $f(t)$, is expressed by the following equation.

$$f(t) = \sum_i \bar{E}_i \lambda_i N_i(t), \tag{5}$$

where

$\bar{E}_i$ = average decay energy of nuclide i,
λ_i = decay constant of nuclide i,
$N_i(t)$ = atomic number of nuclide i.

The average decay energy is divided into the beta ray component ($\bar{E}_{\beta_i}$) and the gamma ray component ($\bar{E}_{\gamma_i}$). The atomic number of nuclide, $N_i(t)$, is given by solving the equation expressing the build-up and decay of the nuclide. In the case of a burst fission, this equation is expressed as:

$$\frac{dN_i}{dt} = -\lambda_i N_i + \sum_j f_{j\to i}(\lambda_j N_j) + y_i, \tag{6}$$

where

$f_{j\to i}$ = production rate of nuclide i,
y_i = independent fission yield for nuclide i.

As seen in the above equation, fission yield data as well as decay data are needed to calculate the decay heat. The fission yield data of the JNDC-V2 library were used in the decay heat calculation. The calculated decay heat has been compared with the measured data.

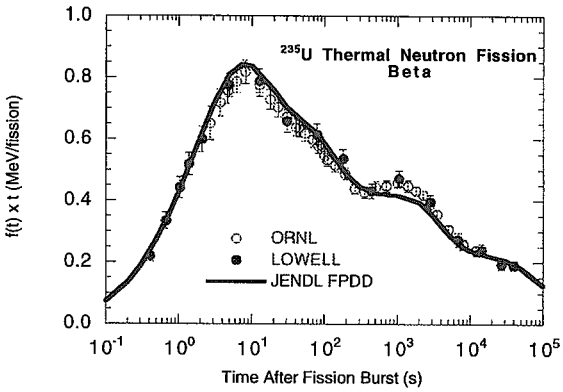

Fig. 3 Beta-ray component of decay heat after ^{235}U thermal neutron fission

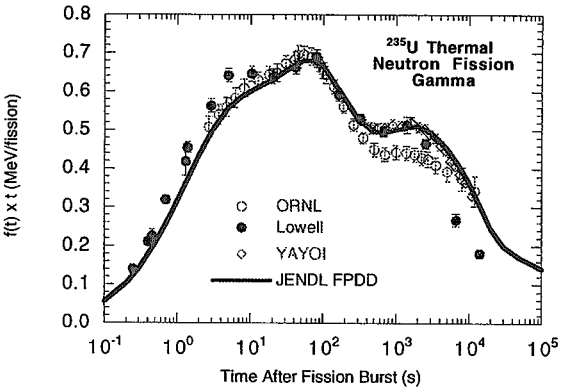

Fig. 4 Gamma-ray component of decay heat after ^{235}U thermal neutron fission

The comparisons have been performed for various kinds of fissionable nuclides. As some examples, the comparisons

of ^{235}U thermal neutron fission and ^{238}U fast neutron fission are shown in **Figs. 3** through **6**. The vertical axes in these figures are the energy release rate multiplied by the time after a burst fission. The beta-ray component and the gamma-ray component are shown separately.

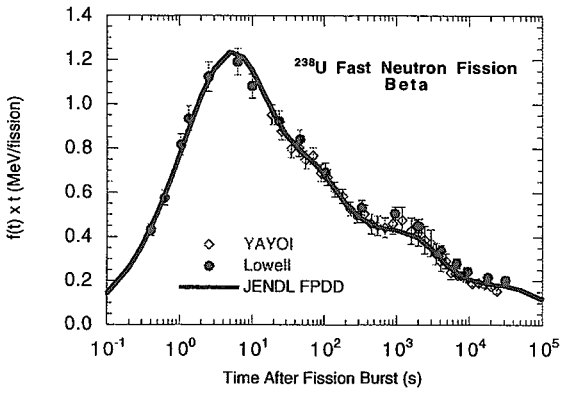

Fig. 5 Beta-ray component of decay heat after ^{238}U fast neutron fission

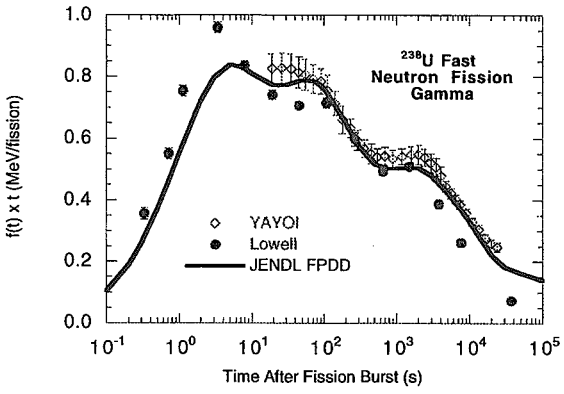

Fig. 6 Gamma-ray component of decay heat after ^{238}U fast neutron fission

Figures 3 and**4** are the beta- and gamma-ray components of ^{235}U thermal neutron fission. The measured data were taken at ORNL[11] and LOWELL.[12] The beta-ray component in **Fig. 3** shows good agreement between the measured data and the calculated values. The LOWELL measurement gives the data at shorter time than 1 s where the nuclides with no or incomplete decay data are main contributor to the decay heat. At the time region the calculated decay heat is consistent with the measured data. This agreement shows that the estimated decay energy values adopted in the JENDL-FPDD file are adequate for decay heat calculation. For the gamma ray component the data from YAYOI[14] are also shown. The YAYOI measurement was performed to check the ORNL data at about a few thousand seconds after a fission where the ORNL data were too small comparing the calculated values. The YAYOI data are different from the ORNL ones but they are consistent with the calculation. The LOWELL data are also different from the ORNL data at this time region but they are also different from the YAYOI data at longer time region where the ORNL and YAYOI data are consistent. Apart from these differences, the calculated results with the JENDL-FPDD file are consistent with the measured data even at the shorter cooling time than 1 second after a fission where the nuclides with the calculated decay data contribute significantly.

Figures 5 and **6** are the beta and gamma ray components of ^{238}U fast neutron fission. The measured data are from LOWELL[13] and YAYOI.[15,16] The calculated results of the beta ray component are consistent with both of the measured data. As for the gamma ray component the calculated results are consistent with the YAYOI data but deviate from the LOWELL data. The inconsistency between the measurements needs to be removed to confirm the reliability of the JENDL-FPDD file.

IV. Spectrum Calculation

The JENDL-FPDD file contains the spectrum data of beta and/or gamma rays of all unstable nuclides as described in Chapter II. The beta and gamma ray spectra of aggregate fission product nuclides have been calculated and compared with the measured data. **Figures 7** through **9** show the comparisons. These figures show the energy spectra.

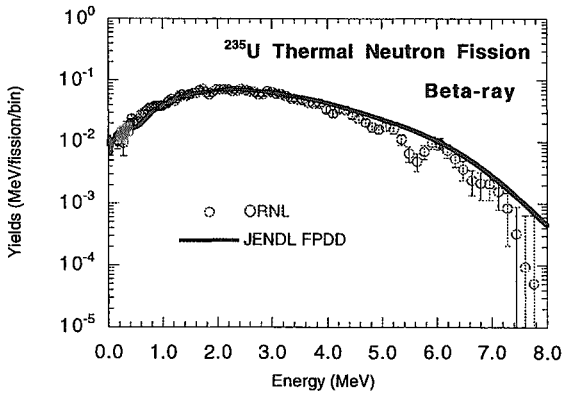

Fig. 7 Aggregate beta-ray spectrum after ^{235}U thermal neutron fission

Figures 7 and **8** are the beta- and gamma-ray spectra after ^{235}U thermal neutron fission. The measured spectra were taken at ORNL.[17] The ORNL spectral data in the figures were measured with the following conditions, that is, 1.0 s irradiation, 1.7 s waiting to start counting and 1.0 s counting. The calculations were performed for a burst fission. The spectrum at time t after a burst fission is approximated to that of finite irradiation of irradiation time t_i, waiting time t_w and counting

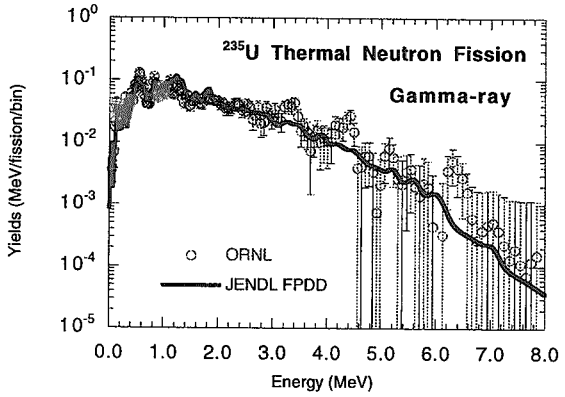

Fig. 8 Aggregate gamma-ray spectrum after ^{235}U thermal neutron fission

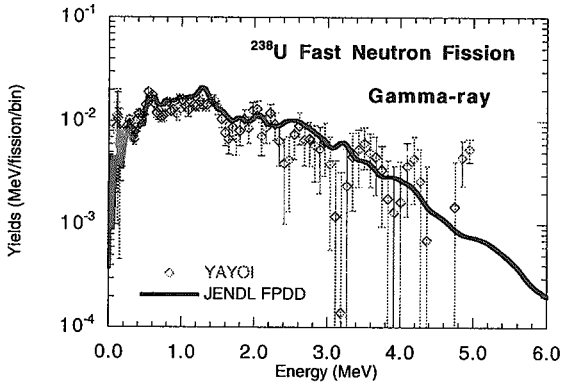

Fig. 9 Aggregate gamma-ray spectrum after ^{238}U fast neutron fission

time t_c when the following relation is maintained:

$$t = t_w + \frac{1}{2}(t_i + t_c). \tag{7}$$

Then the calculated spectra in the figures are those at 2.7 s after a burst fission. In the calculations the detector resolutions are taken into account. The beta-ray spectrum in **Fig. 7** shows good agreement between the measured data and the calculated results although a little bit overestimation is seen at high energy region. The gamma-ray spectrum in **Fig. 8** also shows rather good agreement between the measurement and the calculation. The fine structure at the low energy region is reproduced well although the structure at the high energy region is not seen in the calculation. The failure to reproduce the fine structure at the high energy region is due to the missing of the measured gamma-lines of some nuclides. As seen in **Fig. 2**, the theoretically calculated spectrum is continuous and the line structure is not able to be reproduced. Even though this kind of problem is still remained, the base line of the spectrum seems to be consistent between the measurement and the calculation. This consistency is obtained due to the adoption of the theoretically calculated spectra to the nuclides with no or incomplete spectrum data.

Figure 9 are the gamma-ray spectrum after ^{238}U fast neutron fission. The measured data were taken at YAYOI.[18] As the spectral data of YAYOI has been reported for only gamma-ray spectrum, the comparison of the gamma-ray spectrum is shown here. After 10 s irradiation, the measurement was started at 11 s and the counting was continued for 6 s. The calculation was carried out for a burst fission. Then the calculated spectrum is that at 19 s after a burst fission. The calculated spectrum is in good agreement with the measured one excepting the peak seen at about 5 MeV. This is the same reason as the gamma-ray spectrum of ^{235}U thermal neutron fission.

Although some high energy peaks seen in the gamma-ray spectrum are not reproduced with the JENDL FPDD file as seen in **Figs. 8** and **9**, the general trend of the spectrum is consistent between the measurement and the calculation. When the integration of the spectrum is carried out for whole energy region, the decay heat at the time is obtained. The calculated decay heat from the spectrum becomes to be consistent with the decay heat calculation using the average decay energy values in Chapter III.

V. Summary

JENDL FP Decay Data File 2000 (JENDL-FPDD) has been developed as a special purpose file of JENDL. The JENDL-FPDD file contains the decay data of 1087 unstable nuclides including isomeric states. The theoretically calculated average decay energy values and spectral data are adopted for the FP nuclides with no or incomplete data. The decay heat and spectrum calculations have been performed and compared with the measured data. The comparisons have shown that the JENDL-FPDD file can reproduce the measured decay heat and the beta- and gamma-ray spectra rather well. Using the JENDL-FPDD file, the decay heat and the spectrum calculation will be carried out in a consistent way.

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