Monte Carlo simulation of prompt fission gamma emission

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Abstract

Prompt fission gamma spectra and multiplicities are investigated through the Monte Carlo code FIFRELIN which has been developed recently [1]. Up to now, this code was mainly used to study the characteristics (spectrum and multiplicity) of the prompt neutrons emitted from excited Fission Fragments (FF). When prompt neutron emission is over, the remaining available excitation energy of the FF is assumed to be dissipated as prompt gamma emission. An algorithm, similar to the one used by F. Becvar [2] to treat gamma cascades, has been implemented into the code. It is based on the known discrete levels of the excited fragments as well as on the theoretical models needed to calculate level densities and strength functions. All nuclear structure data are provided by the RIPL3.0 library [3]. Preliminary results relative to gamma deexcitation spectrum and multiplicity for single nuclei are presented. A total gamma spectrum for 252Cf spontaneous fission is also emphasized. Influence of the several methods, models and assumptions on the calculated fission gamma spectra is discussed as well as the prospective for such a simulation.

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1. Introduction

In the context of GEN-III+ reactor conception, calculation of gamma heating in large reflectors must be performed. The gamma part in total heating for such reflectors can reach 90% of the total deposited energy. Needs for accurate gamma production data as well as shortage of such data in JEFF-3.1.1 evaluated files led us to investigate on prompt fission gamma production. In this work, prompt fission gamma spectra and multiplicities are studied through the Monte Carlo code FIFRELIN [1,4]. New features of this code enable us to simulate gamma cascades taking place during the fission process. This article aims to discuss the several hypothesis and models assumed for the gamma evaporation in FIFRELIN simulation. Preliminary results on single isotope deexcitation as well as on the spontaneous fission of 252Cf will be emphasized.
2. FIFRELIN device

The FIFRELIN device aims to simulate the fission fragments evaporation process using Monte Carlo methods and statistical models of the nucleus. A C++ implementation has been chosen giving, among others, the possibility to ensure reliability of the program thanks to unit testing. The simulation of fission for a given nucleus consists of the realization of a great number of fission events. Estimators for interesting observables are incremented during each event so that final results are averaged quantities.

One fission event is simulated through a four major steps algorithm:

• Fission fragments generation: In this phase nuclear mass number, charge and kinetic energy of the fully accelerated primary fragments are sampled.
• Excitation energy calculation: For both fragments, the excitation energy divided in an intrinsic part and a rotational part is calculated based on the total excitation energy released by fission.
• Prompt neutron emission: For both fragments, while the intrinsic excitation energy is high enough, the emission of a neutron is simulated.
• Prompt gamma emission: For both fragments, the remaining excitation energy is then totally dissipated as prompt gamma rays.

Steps 1-3 have already been described in details in Ref.[1]. The gamma emission is new in FIFRELIN and will be the object of the following sections.

3. Gamma cascade model

In the last part of the fragment evaporation process, we assume that only prompt gamma and eventually conversion electrons can be emitted. An algorithm similar to the one used by F. Becvar [2], has been implemented to simulate gamma cascades. The main idea is to build the level schemes of both post neutron fragments up to their excitation energies and then simulate electro-magnetic transitions in those schemes using a Monte Carlo procedure.

3.1. Level scheme build

A reachable excited level for a nucleus is characterized by its energy and its spin parity. In order to build a complete level scheme for a considered post neutron fragment, two energetic domains are distinguished separated by a energy cutoff. Under this energy cutoff, a complete set of levels is provided by the RIPL3.0 data library taking into account experimental transitions measurements. Those levels are used with no modifications and form the low energy part of the level scheme.

Above the cutoff energy, not only levels given by RIPL3.0 may not have spin-parity information but also their cumulated number becomes insufficient as excitation energy increases. To build the high energy part of the level scheme, the first operation consists in completing RIPL3.0 levels data. Unknown spin-parities are sampled using the following probability law:

\[
P(J, \pi) = 0.5 \cdot \frac{2J + 1}{2\sigma^2} \cdot \exp \left( -\frac{(J + 1/2)^2}{2\sigma^2} \right)
\]  

(1)
An energy dependant spin cutoff $\sigma^2$, as described in RIPL3.0 manual [3] for the back shifted Fermi gas model of level density, has been used. The level density parameter required follows the Ignatyuk formulation [5] with Myers-Swiatecki shell corrections [6]. The second operation consists in adding new levels with sampled energy and spin-parity such that our scheme is coherent with a chosen theoretical level density (see Fig.1). Implemented level density models are the constant temperature model (CTM) [3] and the composite Gilbert-Cameron model (CGCM) [7].

![Figure 1: Cumulated number of levels for $^{144}$Ba](image)

3.2. Gamma emission

Once the post neutron fragment excitation energy and complete level scheme are established, gamma cascades can be simulated. First of all, the starting level for the cascade is sampled between the two levels with energy closest to the fragment excitation energy. Probabilities allowed to both levels are classically determined so that average starting energy corresponds to the fragment excitation energy. Then several gamma-ray emissions are simulated until the ground state is reached by using the following algorithm:

- Determine probabilities for every possible gamma or conversion electron transitions to down levels.
- Sample one of those transitions and decay to the target level.
- Record emitted particle data (energy $\epsilon_\gamma$, multipolarity $XL$, multiplicity $M_\gamma$ ...).

Probabilities of transitions for prompt gamma are either directly taken from RIPL3.0 data library if available or calculated based on gamma strength functions ($f_{XL}$) as following:

$$P(\epsilon_\gamma, XL) = \frac{y_{XL}^2 \cdot f_{X\gamma}(\epsilon_\gamma) \cdot \epsilon_\gamma^{2L+1}}{N}$$

(2)

In equation (2), the denominator N corresponds to a normalisation factor. The $y$ term accounts for the Porter-Thomas fluctuation and is sampled in a normal distribution so that its square respects a chi-squared probability distribution with one degree of freedom. For E1 transitions, the standard lorentzian (SLO) or the enhanced generalized lorentzian (EGLO) as described in [3] has been used. An approximation has been assumed for M1 and higher transition multipolarities, which have been described as following:
If a conversion coefficient is available in the RIPL3.0 input data library, the internal conversion is taken into account and an electronic transition is made possible.

4. Preliminary results

4.1. Deexcitation of a single nucleus

To obtain a converged gamma deexcitation spectrum for a single nucleus, 100 batches of 1000 cascades have been processed. The level scheme used for gamma cascades is built at the beginning of each batch following the procedure described in the previous section. During the batch the primary transitions are stored in memory to reduce time calculation whereas secondary transitions are evaluated each time it is necessary. In this part a CTM level density has been chosen whereas the E1 strength function follows the enhanced generalized lorentzian model.

The figure 2a shows the gamma emission spectrum obtained from a 3 MeV excited $^{144}$Ba post neutron fragment. The scheme up to 3 MeV was formed of 316 levels so that a bump appears in the spectrum between 0.5 and 2.5 MeV. First discrete levels close to the ground state are responsible for the discrete rays. The 199 keV gamma line can be identified as the transition from the first excited level to the ground state.

We also tested our code simulating a 10 keV neutron captured by $^{55}$Mn. Considering only s-wave neutrons the initial spin-parity of the excited compound nucleus $^{56}$Mn has been forced to be 2$^-$ or 3$^-$. Spectra for both initial spin-parity have been calculated and were found very similar. As a consequence, we built the $^{55}$Mn capture spectra assigning a 0.5 probability for each possible spin-parity. Figure 2b compares our results with the 10 keV neutron capture of $^{55}$Mn spectrum provided by JEFF-3.1.1. The global shape of the spectrum is well reproduced in spite of a slight overestimation of the 1 to 3.5 MeV gamma emission probabilities.
4.2. $^{252}\text{Cf}$ spontaneous fission

The $^{252}\text{Cf}$ spontaneous fission has been simulated processing $10^5$ fission events. For every post neutron fragment generated, the level scheme is built up to the remaining excitation energy and one gamma cascade is simulated. A CGCM level density has been used based on Ignatyuk formulation for the level density parameter. Shell corrections are taken from Myers-Swiatecky calculation [6]. Unknown gamma transitions are derived from a EGLO strength function for the E1 multipolarity with parameters provided by RIPL3.0 files or systematics. The total spectrum is represented on figure 3 in comparison with former experimental results. The Verbinski [8] and Van der Ploeg [9] data have been directly scanned from original publications. In the Hotzel et al. publication [10], several spectra are given for sorted fragmentation. Here, Hotzel’s total spectrum has been derived by weighting those spectra by their respective mass yield taken from Varapai’s measurement [11]. Those yields have been chosen because they are already used in the fission fragment mass sampling in FIFRELIN.

![Figure 3: Comparison of the calculated prompt gamma spectrum for the $^{252}\text{Cf}$ spontaneous fission with experimental data](image)

| Reference                  | $M_\gamma$ | $<\varepsilon_\gamma>$ (MeV) | $<E_\gamma>$ (MeV) |
|----------------------------|------------|-------------------------------|-------------------|
| Nifenecker, et al. (1972) [12] | 7.75       | 0.88                          | 6.84              |
| Verbinski, et al. (1973) [8] | 7.80       | 0.88                          | 6.84              |
| Nardi, et al. (1973) [13]    | /          | /                             | 6.7 ± 0.4         |
| This work                  | 5.87 ± 0.01| 1.05                          | 6.43 ± 0.01       |

This preliminary calculation results in a spectrum not so far from previous measurements. The bump in the Verbinski data around 1.3 MeV is reproduced and seems to come from several discrete rays. However, a bump in the gamma emission with energy higher than 2 MeV is observed in the calculated spectrum and not in the experiments. The low value of average gamma multiplicity given in table 1 and compared with former measurement is consistent with the too hard spectrum observed.
4.3. Influence of level density and strength function models

The $^{252}$Cf prompt fission gamma spectrum has been calculated using different models of level density and E1 strength function. Results are shown in figure 4 with a resolution of 100 keV. It seems that prompt gamma spectrum is highly sensitive to level density modifications whereas E1 strength function plays less important role. The bump in gamma emission with energy higher than 2 MeV has been decreased by the use of the CTM. This may be explained by the great number of levels for high excitation energies provided by the CTM model, that improve low energy transitions. The simulation with a CTM level density gave an average gamma energy of 0.95 MeV, which is still high compared to experimental results. This study shows that a particular attention must be paid to the parameterisation of the level density.

![Figure 4: Prompt gamma spectra for $^{252}$Cf spontaneous fission (resolution = 100 keV) calculated using different models (see text)](image)

5. Perspectives and Conclusion

The implementation of gamma cascade simulation methods has been realized and can be applied to a vast domain of nuclei. Several models for various nuclear quantities (level density, strength function, spin cutoff, density parameter...) have been described in the code in view to investigate their influence on prompt gamma spectra and multiplicities. Application of gamma cascade process to FIFRELIN fission simulation provided preliminary prompt gamma spectra for the $^{252}$Cf spontaneous fission. Those results reproduce the global shape of Verbinski’s data [8] but overestimate the emission of high energetic gamma rays ($\varepsilon_\gamma > 2$MeV). It has been shown that a part of this overestimation could come from parameters and models of the level densities used for the calculation.

For the future, improvement of the code must be realized to perform calculation using less time and memory. Then an investigation on level density parameterization will be considered, as well as a sensitivity study of gamma multiplicity and spectrum to several model parameters. At last, those methods will be applied to provide gamma production data for spontaneous and induced fission of main fissile isotopes.
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