Progress in NUCLEAR SCIENCE and TECHNOLOGY, Vol. 2, pp.757-761 (2011)

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Particle-Gamma and Particle-Particle Correlations in Nuclear Reactions Using Monte Carlo Hauser-Feshbach Model

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Monte Carlo simulations for particle and γ-ray emissions from an excited nucleus based on the Hauser-Feshbach statistical theory are performed to obtain correlated information between emitted particles and γ-rays. We calculate neutron induced reactions on ^{51}V to demonstrate unique advantages of the Monte Carlo method, which are the correlated γ-rays in the neutron radiative capture reaction, the neutron and γ-ray correlation, and the particle-particle correlations at higher energies. It is shown that properties in nuclear reactions that are difficult to study with a deterministic method can be obtained with the Monte Carlo simulations.

KEYWORDS: nuclear reaction, nuclear data, statistical model, Monte Carlo method

I. Introduction

Nuclear data are essential ingredients in radiation transport simulations, which provide all probabilities of interactions (cross sections) between materials and the particles and photons of interest. A complete set of evaluated nuclear data requires not only the reaction cross sections but also energy and angular distributions of emitted particle, γ-ray production cross sections, and so on. This information of nuclear reaction, in which some of them are often inaccessible experimentally, is given by theoretical model calculations, such as the optical model, the statistical Hauser-Feshbach model,[1] and the pre-equilibrium model.

Despite the fact that the nuclear reaction models provide a set of consistent physical quantities, it is very difficult to utilize the whole information due to limitations in the database file format and application codes. Moreover, the nuclear reaction codes, such as GNASH,[2] EMPIRE,[3] and TALYS,[4] do not produce correlations among the emitted particles and γ-rays explicitly. The correlations can be a signature of a particular nuclear reaction occurred in a nuclear system. With a transport simulation that utilizes the correlated particle emissions for the system, we will be able to probe that system in more microscopic way.

In this study we perform Monte Carlo simulations for particle and γ-ray emissions to obtain the correlated information among the emitted particles and γ-rays. The particle and γ-ray production probabilities are calculated with the Hauser-Feshbach statistical theory[1] and the pre-equilibrium model. We have been developing a new computer code to solve the Hauser-Feshbach equation with the Monte Carlo method,[5] which basically simulates real nuclear reactions occurring inside a nucleus event-by-event. This technique allows us to explore wider application areas in the future, such as correlations between emission energies and neutron multiplicities in the prompt fission neutrons,[6–9] recoils and kerma for calculations of energy deposition and damage, and so on.

II. Monte Carlo Hauser-Feshbach Method

1. Particle and γ-Ray Emission Probabilities

Figure 1 schematically shows sequential neutron emissions for the system n+(Z, A), including γ-ray emissions. We first need to define a decay probability from a given compound state (c_n, k_n), where c_n denotes the compound nucleus (c_0 for the compound nucleus $(Z, A+1)$ in Fig. 1), k_n is the index of excited state with the energy bin width of ΔE, and the suffix n describes the n-th compound nucleus. The index k runs from the highest excitation toward the ground state. For example, (c_0, k_0) is the highest excited state in the initial compound nucleus. We define a probability $P(c_n, k_n, c_m, k_m)$, which is a decay probability of the state (c_n, k_n) by emitting a particle or a γ-ray to form a (c_m, k_m) state. The probability also requires indices of the spin and parity for both initial and final states. However we employ $P(c_n, k_n, c_m, k_m)$ in such a way that all the transitions that satisfy the spin and parity selection rule are already summed, so that P only depends on the energy difference k_n and k_m, and the particle energy is calculated as $(k_m - k_n)\Delta E$. The probability P can be calculated with the Hauser-Feshbach theory,[1]

$$P(c_n, k_n, c_m, k_m) = \frac{T(c_m k_m \to c_n k_n)}{\sum_{c_m k_m} T(c_m k_m \to c_n k_n)}, \quad (1)$$

where $T(c_m k_m \to c_n k_n)$ is the particle or γ-ray transmission coefficient from the final (c_m, k_m) to initial (c_n, k_n) states. The sum in the denominator ensures the proper normalization. The particle transmission coefficients are obtained by solving the Schrödinger equation for optical model potentials, and the γ-ray transmission coefficient is calculated from the γ-ray strength function in a standard manner.[10)]

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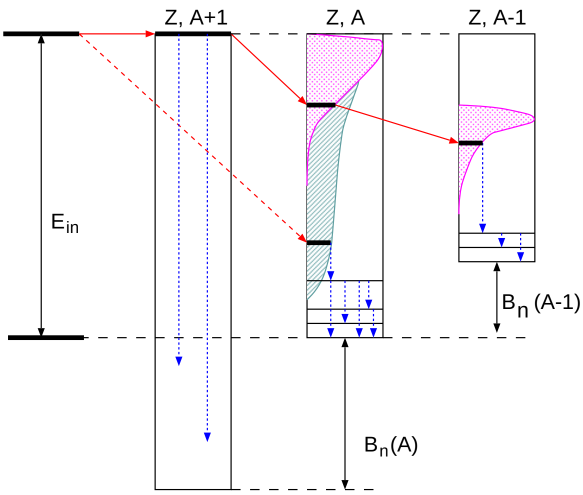

Fig. 1 Schematic picture of multiple neutron emission process for the neutron induced reaction on the target (Z, A). The solid arrows are the compound nucleus decay by neutron emission, the dashed arrow is the pre-equilibrium process that does not form a compound nucleus $(Z, A+1)$, and the dotted arrows are the γ-ray emission. The vertical scale represents nuclear excitation, B_n is the neutron binding energy.

2. Monte Carlo Technique

Once the probabilities $P(c_n, k_n, c_m, k_m)$ are constructed with the Hauser-Feshbach formula, a Monte Carlo simulation for the particles and γ-ray decay processes is straightforward. Starting with the initial state (c_0, k_0), a following state can be determined by throwing a dice based on the probability $P(c_0, k_0, c_1, k_1)$, where we know that

$$\sum_{c_1 k_1} P(c_0, k_0, c_1, k_1) = 1. \qquad (2)$$

Once the next nuclear state (c_1, k_1) is chosen, the probabilities P from (c_1, k_1) are calculated by Eq. (1) again. We repeat this random sampling procedure until the nucleus reaches a stable state, and record all the particles and γ-rays emitted during the sequence.

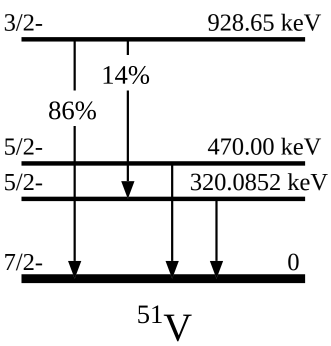

Fig. 2 Excited states of ^{51}V below 1 MeV, and the γ-decay probabilities from these levels.

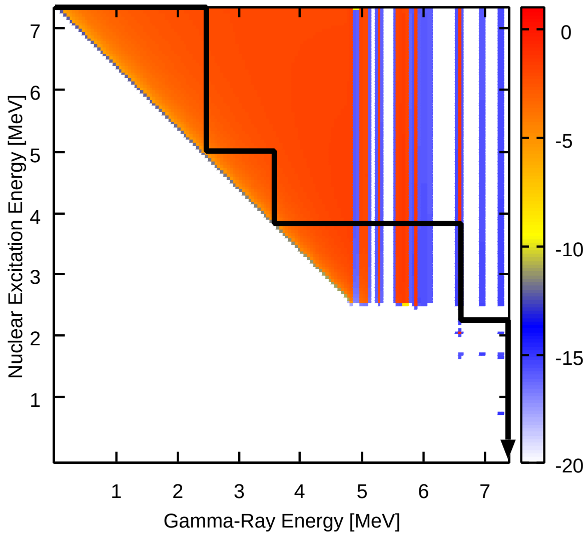

Fig. 3 The γ-decay probability matrix from a 100 keV neutron capture state of ^{52}V*. The vertical axis represents the excitation energy, and the horizontal axis is a relative energy of emitted γ-rays. The transition probabilities (in log) are shown by the color scale.

3. Hauser-Feshbach Model Calculation

The CoH Hauser-Feshbach code version 3.1, CoH_3[11], calculates all the nuclear reaction cross sections above the resonance range, including the total, shape elastic scattering, direct inelastic scattering, direct/semidirect capture cross section, pre-equilibrium emission, and particle and γ-ray emission in the nuclear decay process. The main ingredients in the Hauser-Feshbach model calculation are the optical model potentials for neutron and charged particles, the level density parameters, the γ-ray strength function, and the discrete level properties for all residual nuclei. In this study we adopt the Koning-Delaroche global optical potential[12] for neutron and proton, the α-particle optical potential of Avrigeanu et al.,[13] the generalized Lorentzian form for the γ-ray strength function of Kopecky and Uhl,[10] the composite level density formulae of Gilbert and Cameron[14] with an updated parameterization.[15] The discrete level data are taken from RIPL-3.[16]

III. Results and Discussions

1. γ-Ray Correlation for Neutron Radiative Capture

As an example, we consider a 100-keV neutron induced reaction on ^{51}V. The neutron separation energy for ^{52}V is 7.31 MeV. The energy bin width ΔE in this calculation is 50 keV. Because the first excited state of ^{51}V is 320 keV, shown in **Fig. 2**,[16,17] the compound nucleus ^{52}V* decays by emitting several γ-rays (neutron radiative capture) or by emitting a neutron leaving the residual ^{51}V in its ground state (compound elastic scattering). The calculated γ-ray emission probability matrix is shown in **Fig. 3**. The initial neutron captured state in this figure is the left top corner, and a first γ-ray emission takes place along the horizontal line from there, under the probability distribution represented by the different colors. After the γ-ray emission, the second γ-ray is emit-

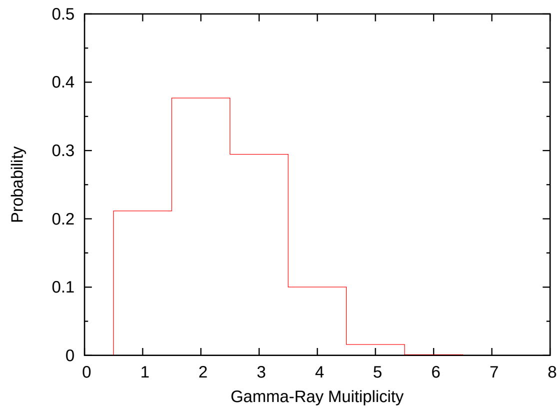

Fig. 4 The γ-ray multiplicity distribution for the 100 keV neutron capture reaction.

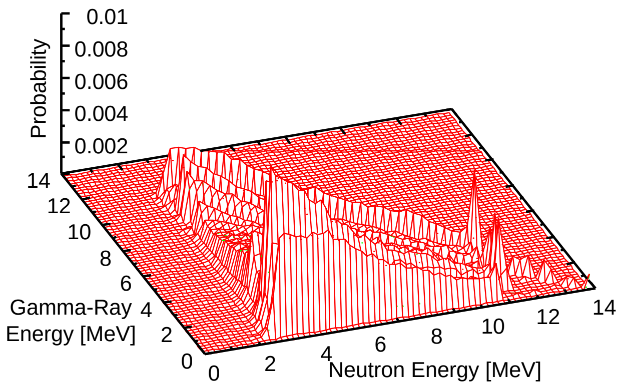

Fig. 5 Correlation between a neutron and γ-rays emitted from the ^{51}V(n,n') reaction at $E_n = 14$ MeV. The z-axis is a probability per neutron inelastic scattering.

ted from the corresponding energy state. The thick black line shows a typical γ-ray cascade path, in which the γ-ray multiplicity is four.

The Monte Carlo simulation for the γ-ray cascading can be performed once the matrix in Fig. 3 is provided. In **Fig. 4** shows the γ-ray multiplicity distribution. The average multiplicity $\langle m \rangle$ calculated from this distribution is 2.33.

The average multiplicity can be calculated with the deterministic method. The average γ-ray energy is given by

$$\langle E \rangle = \frac{\displaystyle\int_0^\infty E\phi_\gamma(E)dE}{\displaystyle\int_0^\infty \phi_\gamma(E)dE}, \qquad (3)$$

where $\phi_\gamma(E)$ is the γ-ray energy spectrum, and therefore

$$\langle m \rangle = \frac{E_{n,\mathrm{cms}} + B_n}{\langle E \rangle}. \qquad (4)$$

From Eq. (4), $\langle E \rangle = 2.34$, which is close enough to the Monte Carlo result of 2.33. The deterministic method, however, cannot provide the distribution of m like in Fig. 4, in contrast, the Monte Carlo technique facilitates access to individual γ-ray multiplicities and their energy distributions.[5)]

2. Neutron and γ-Ray Correlation at 14 MeV

Except for strong direct transitions to low-lying states, cross sections for neutron inelastic scattering is one of the most difficult process to measure experimentally, because a single neutron emission event has to be discriminated from all other neutron emission processes, such as (n,2n) and (n,np) reactions. An activation technique is inadequate, as the residual nucleus returns to the stable ground state after prompt γ-ray emissions. Recent advanced experimental technique to measure the inelastic scattering cross section is a coincidence experiment, *i.e.* a scattered neutron detection gated by a particular γ-ray transition, such as a prominent γ transition from the first excited to the ground states.

The Monte Carlo simulation tells us how the pure (or exclusive) neutron inelastic scattering process can be related to the γ-ray emissions, including the γ-ray multiplicities and their energy spectra. The joint probability for the energies of inelastically scatterer neutrons and γ-rays is shown in **Fig. 5**. The probability is normalized per neutron emission, which means γ-ray multiplicities are implicitly included (an inelastic scattering process produces several γ-rays). Low energy neutrons are not observed, because the most likely process there is the (n,2n) reaction (Q-value for (n,2n) is -11 MeV). The γ-ray energy spectra are constrained by the emitted neutron that removes the excitation energy of the compound nucleus. The lower the neutron energy is, the harder the γ-ray spectrum with the larger multiplicity becomes, and vice versa, which satisfies the energy conservation.

After the excited ^{51}V* is produced in the inelastic scattering process, it decays by emitting several γ-rays to reach at the ground state. This γ-ray cascading often produces strong γ-ray lines in the energy spectrum, which are transitions between the low-lying states, depicted by the arrows in Fig. 2. In fact, the 320-keV γ-line is seen in Fig. 5. Although an evaluation in Table of Isotopes[17)] does not have the 470 keV line, we followed RIPL-3[16)] to include this level too.

When we perform an experiment to measure the inelastic scattering cross section by detecting the 320-keV γ-ray, we have to correct the measured cross section by adding the unseen partial cross section that bypasses the 320 keV transition. This correction can be made by calculating the energy spectra for both cases — the total neutron spectrum, and the partial spectrum that is obtained by gating on the 320-keV γ-line. The calculated spectra are show in **Fig. 6**. The spectra are normalized to $\sigma_{n'}/\sigma_R$, where $\sigma_{n'}$ is the total inelastic scattering cross section and σ_R is the total reaction cross section. The coincidence measurement obviously lower the statistics, and it is shown in Fig. 6 that only 17% of the total inelastic scattering process produces the 320-keV γ-line in the case of ^{51}V(n,n') reaction at 14 MeV.

The ratio of two cases above depends strongly on the level structure and the evaluated γ-ray branching ratios. For example, an even-even nucleus, which manifests a rotational band structure of 0^+-2^+-4^+, tends to yield a clean $2^+ \to 0^+$ discrete transition γ-line.[18)] The Monte Carlo Hauser-Feshbach method predicts all the γ-lines that are inherent to a reaction of

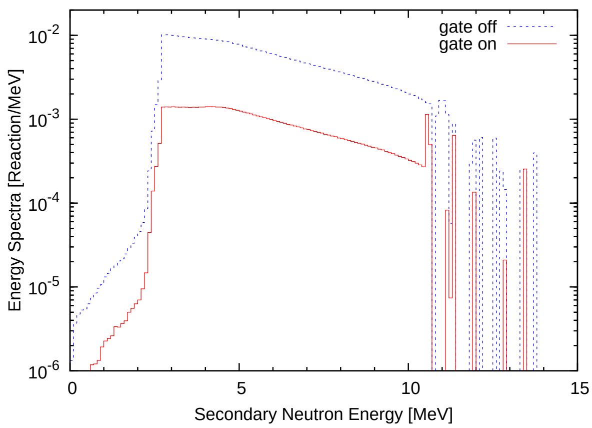

Fig. 6 Calculated neutron energy spectra for the inelastic scattering process at 14 MeV. The dashed line is for the total energy spectrum, and the solid line is only neutrons that produce the 320-keV γ-ray.

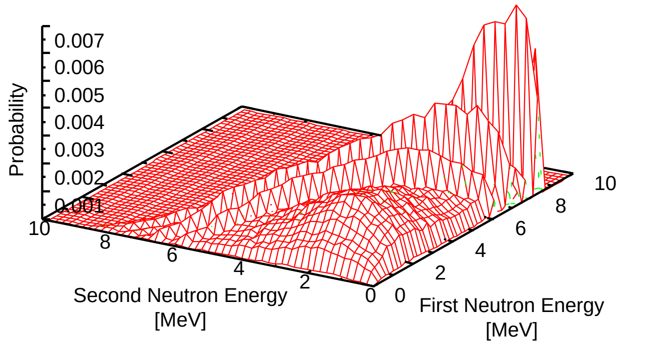

Fig. 7 Correlation between two neutrons emitted from the ^{51}V(n,2n) reaction at $E_n = 20$ MeV. The z-axis is a normalized probability.

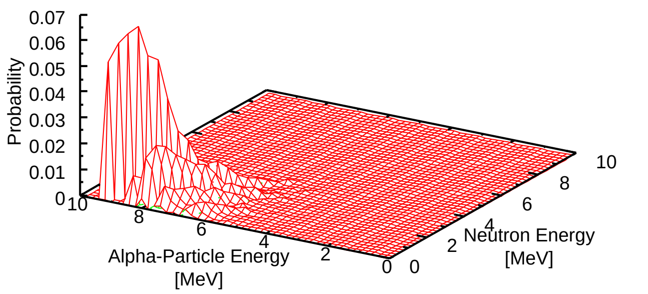

Fig. 8 Correlation between a neutron and an α-particle emitted from the ^{51}V(n,nα) reaction at $E_n = 20$ MeV.

interest, although the calculation is suffered by uncertainties in the nuclear structure data in some cases.

3. Nuclear Reactions at 20 MeV

For the 20-MeV neutron induced reactions, (n,n'), (n,p), (n,α), (n,2n), (n,np), (n,nα), and (n,pα) reaction channels open. We ignore emissions of the other charged particles, such as deuterons, because their cross sections are too small. The statistical Hauser-Feshbach model gives energy spectra of emitted particles and γ-rays, $\phi_n(E)$, $\phi_p(E)$, $\phi_\alpha(E)$, and $\phi_\gamma(E)$ for each compound nucleus.

In the case of (n,2n) reaction, the two emitted neutrons have different energies, and there is a correlation between these energies. We generated the joint probabilities $p(E_1, E_2)$, where E_1 and E_2 are the energies of first and second neutrons, and the normalized probability distribution is shown in **Fig. 7**. The probability is distributed in the $E_1 + E_2 \leq 8.56$ MeV triangular area, because E_1 and E_2 cannot exceed the maximum energy of ^{50}V*. The probability distribution has some structure when $E_1 > E_2$. Since the first neutron removes a lot of initial excitation energy from the $A+1$ system, the final states of the second neutron emission are often in the discrete levels, and this causes the structure in Fig. 7. In general, the first neutron tends to carry more energy than the second one, and this can be understood by the fact that the nuclear reaction at the initial stage is governed by the pre-equilibrium process.

Figure 8 shows the energy correlation between the emitted neutrons and α-particles for the (n,nα) reaction. The plotted joint probability is the sum of (n,nα) and (n,αn) processes. Because the emission of the low energy α-particle is strongly suppressed by the Coulomb barrier, the α-particle spectrum becomes much harder than the neutron spectrum. The Monte Carlo Hauser-Feshbach model takes all this kind of physical requirements into account automatically. Unfortunately, the calculated correlations cannot be fully utilized in radiation transport simulations, due to difficulties in making transport libraries. One of the extreme applications of our technique is to use the Monte Carlo Hauser-Feshbach code as an event generator in the radiation transport code. This may require a high performance computer, because all the probabilities of particle and γ-ray interactions are calculated on-the-fly. Nevertheless we believe this could be feasible in near future, owing to recent advances in computer science. This does not mean we don't need the transport libraries anymore, since the Hauser-Feshbach theory is incapable to predict resonances. Our developed method can be an alternative way to feed a set of nuclear data above the resonance region into the radiation transport codes.

IV. Conclusion

We performed Monte Carlo simulations for particle and γ-ray emissions in nuclear reactions to demonstrate unique advantages of the method for investigating correlations among the emitted particles and γ-rays. The decay probabilities at each compound state are calculated with the Hauser-Feshbach statistical theory with the pre-equilibrium emission. Calculated results for the neutron induced nuclear reactions on ^{51}V were shown as examples, which were the correlated γ-rays for the neutron radiative capture reaction at a low energy, the neutron and γ-ray correlation, and the particle-particle correlations at higher energies. These quantities are very difficult to extract from the nuclear model calculations with traditional methods, nevertheless the correlations between different processes bring us new insights into the nuclear reaction. The Monte Carlo Hauser-Feshbach technique described in this paper sheds light on concealing nuclear reaction mechanisms at first time.

Acknowledgment

This work was carried out under the auspices of the National Nuclear Security Administration of the U.S. Department of Energy at Los Alamos National Laboratory under Contract No. DE-AC52-06NA25396.

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