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ARTICLE

Application and Validation of Event Generator in the PHITS Code for the Low-Energy Neutron-Induced Reactions

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The "Event Generator Mode (E-mode)" has been introduced into the Particle and Heavy Ion Transport Code Systems (PHITS) in the treatment of transport phenomena of low energy neutrons below 20 MeV. In E-mode, the evaluated nuclear data for neutron-induced reactions and a special statistical decay model are combined so as to trace all correlations of ejectiles and residuals in a collision under the energy and the momentum conservation. For the validation of the E-mode below 20 MeV, we have calculated neutron-induced activation cross sections and double differential cross sections by the E-mode, and compared them with the experimental data and the evaluated nuclear data library such as ENDF/B-VII and JENDL-4. As results, calculated results for neutron emission reproduced the data well, but there was small discrepancy between calculated results for charged particle emission and the evaluated nuclear data. As an application of this mode, we indicated new calculations about the energy distributions of charged particles for the ^{10}B(n_{th}, α)^{7}Li and 24 keV ^{6}Li(n, α)t reactions. In future, E-mode of PHITS will be modified and applied to the analysis of the biological effects, the single setup error of semiconductor, and many other fields.

KEYWORDS: event generator, Monte Carlo, low-energy neutron incidence, PHITS, energy distribution

I. Introduction

The concept of the event generator is rather popular with the Monte Carlo simulation code for high energy particles. In the event generator mode, the conservation law on the energy and the momentum is sustained in each event. Recently, the correlated quantities such as event-by-event distribution of deposit energy even in low energy fields are often required for microdosimetric estimations of irradiation effects in biology and semiconductors. For these requirements, the "Event Generator Mode (E-mode)[1)]" has been introduced into the PHITS code[2)] in the transport of low energy neutrons. In this mode, the evaluated nuclear data for neutrons and a special statistical decay model are combined so as to trace all correlations of ejectiles keeping the energy and the momentum conservation in a collision. This mode enables us to calculate the correlated quantities mentioned above, and also to estimate the activation cross section, the Kerma coefficient and the displacement cross section data without additional evaluated cross section libraries. The validation of E-mode for the Kerma coefficient and the displacement cross section was presented in the other proceedings.[3)]

For the validation of E-mode in neutron-induced reactions under 20 MeV, we have calculated low energy neutron-induced activation cross sections and charged particle production cross sections by E-mode, and compared them with the experimental data and the evaluated nuclear data library such as ENDF/B-VII[4)] and JENDL-4.[5)] As an application of this mode, we have suggested a new approach to the energy distribution for the thermal and 24 keV neutron incident reactions on boron and lithium-6.

II. Method of Calculations

A brief flowchart of the Event Generator Mode is shown in **Fig. 1**. A detail is presented in the other paper.[1)] The evaluated nuclear data of the total cross section, and the channel cross sections, i.e. capture, elastic and (n,n'), (n,Nn) cross sections, are used for branching the reactions, and the double differential cross sections of outgoing neutrons are used for the spectrum of the first emitted neutron.

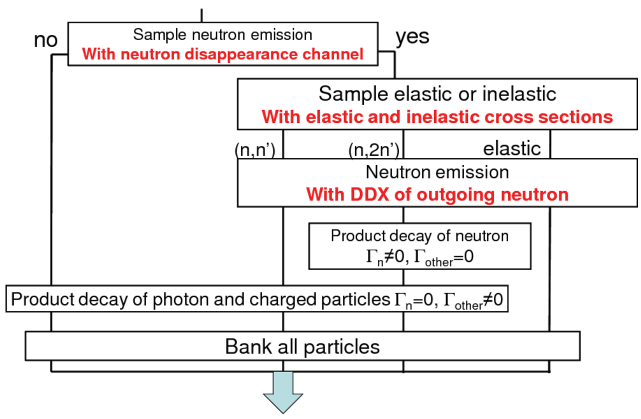

Fig. 1 A brief flowchart of the Event Generator Mode. Energy and momentum are conserved in an event.

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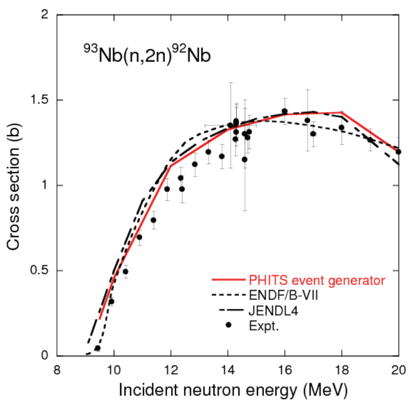

Fig. 2 Activation cross section for the ^{93}Nb(n,2n)^{92}Nb reaction. All experimental data were taken from the web site of NNDC[6].

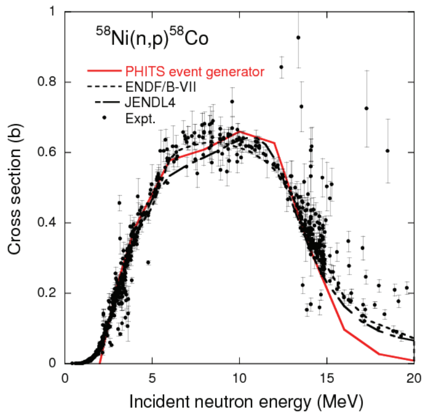

Fig. 3 Activation cross section for the ^{58}Ni(n,p)^{58}Co reaction. All experimental data were taken from the web site of NNDC[6].

We categorize the channels by the number of outgoing neutrons. For the channel which does not produce neutron, we call this "neutron disappearance channel", the excitation energy and momentum of neutron-captured nucleus is determined uniquely from the incident energy of neutron and target nucleus. For the decay process of this excited nuclei, the special statistical decay model in which the dcay width of neutron is assumed to be zero, is applied. Then all information of ejectiles, in this case, charged particles, photon and residual nucleus can be determined.

For an elastic reaction, the scattering angle of outgoing neutron is determined according to the nuclear data. By the kinematics of this elastic channel, the energy of neutron and the momentum of the residual nucleus can be determined uniquely.

For (n,n') reactions, the momentum of outgoing neutron is determined according to the double differential cross section of the nuclear data. By the kinematics of this emission, the excitation energy and momentum of the residual nucleus are determined uniquely. Next, the special statistical decay process without neutron emission width is also applied.

Finally, for (n,Nn') reaction, a similar way as in the (n,n') case is applied, but after one neutron emission, the special statistical decay process with only neutron emission width is adopted until N nucleons are emitted. After this, the special statistical decay process without neutron emission width is applied. By these processes, we can treat a low energy neutron collision as an "event", which means the energy and momentum are conserved in an event. Therefore, by this mode, we can extract any information, e.g. the kinetic energy distribution of the residual nuclei, two-particle correlation, etc in the transport calculation of PHITS.

III. Validation of E-Mode

In the procedure of E-mode, the total cross section, the branching ratio of each reaction channels and the neutron production double differential cross sections are taken from the nuclear data library. The other information, which is necessary to determine all ejectiles of the reaction in an event, is complemented by the special statistical decay model. We do not use the production cross sections of charged particle,

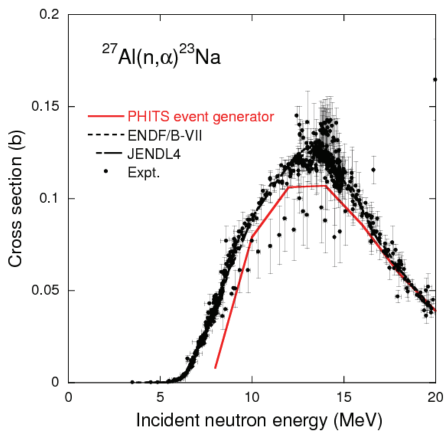

Fig. 4 Activation cross section for the ^{27}Al(n,α)^{23}Na reaction. All experimental data were taken from the web site of NNDC[6].

residual nuclei, nor photon included in the nuclear data library. Therefore, the evaluated charged particle production cross section in the nuclear data library may be different from the results obtained by E-mode in PHITS. So it is important to compare these production cross sections between the calculated results obtained by E-mode and the evaluated nuclear data. In this section, we have indicated the validation of E-mode for the activation cross section and the charged particle double differential cross section by showing comparisons between calculated results of E-mode and evaluated nuclear data such as ENDF/B-VII and JENDL-4, and also experimental data. JENDL-3.3 was employed for the calculation of E-mode. Experimental data were taken from the web site of National Nuclear Data Center (NNDC) in Brookhaven national laboratory.[6]

1. Activation Cross Section

Neutron induced activation cross section is important for the estimation of radioactivity in facilities of accelerator and nuclear power plant. Therefore, the evaluated nuclear data library for the activation cross section has been made using many experimental data. In **Figs 2-4**, we have compared the calculated results with evaluated nuclear data library of ENDF/B-VII and JENDL-4 and experimental data for the

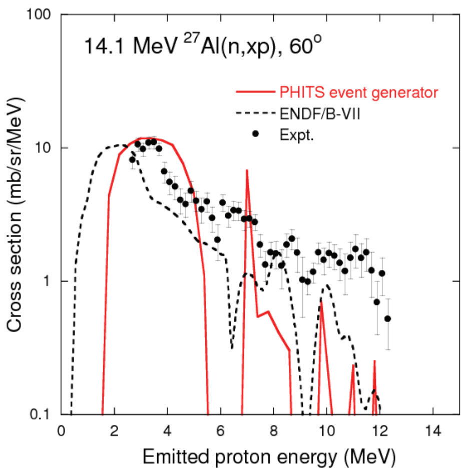

Fig. 5 Double differential cross section for the ^{27}Al(n,xp) reaction at 60°. Experimental data were taken from Reference 7.

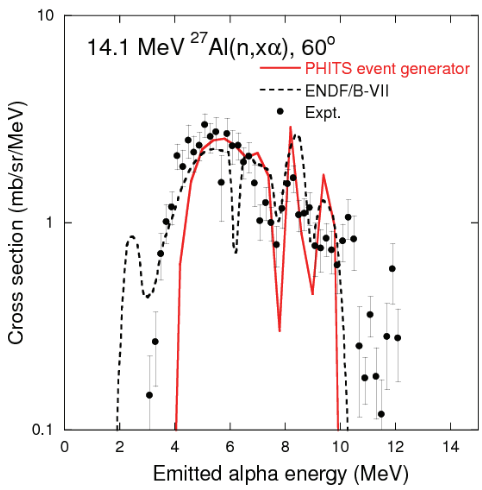

Fig. 6 Double differential cross section for the ^{27}Al(n,xα) reaction at 60°. Experimental data were taken from Reference 7.

^{93}Nb(n,2n)^{92}Nb, ^{58}Ni(n,p)^{58}Co, and ^{27}Al(n,α)^{23}Na reactions.

Calculated results for the ^{93}Nb(n,2n)^{92}Nb reactions agree very well with the evaluated nuclear data and experimental data. The results for the ^{58}Ni(n,p)^{58}Co and the ^{27}Al(n,α)^{23}Na reactions slightly disagree with the ENDF/B-VII data. The reason for this discrepancy might be that all charged particles are produced by the special decay process in a statistical way in E-mode. The other reaction mechanisms such as a preequilibrium emission and break up processes are necessary to improve this situation.

2. Double Differential Cross Section

For the evaluation of the heat in the material, an important thing is the kinetic energy distribution of charged particles and photons produced by a collision. As mentioned earlier, only the first neutron production double differential cross section is taken from the nuclear data and the other cross sections such as charged particle and photon are described by E-mode. Therefore, it is important to compare the calculated results using E-mode with evaluated nuclear data for the charged particle and photon production. **Figures 5-7** show calculated double differential cross sections of the proton, alpha and photon productions for the 14.1 MeV and 9.5 MeV neutron incident reactions and comparisons to ENDF/B-VII and experimental data.[7,8] For the proton, alpha and photon productions, calculated results of E-mode as well as ENDF/B-VII data have shown discrete levels although experimental data is almost continuum due to the contribution of the energy resolution of detectors. In E-mode, we have taken into account the discrete levels near the ground state of nucleus in the special statistical decay process, but we do not consider the characteristic of each level for the transition but only by a statistical way. These might be the reasons that calculated results show discrete levels but the strength of some peaks of the results differs from the data. It is also noted that the hybrid treatment of both nuclear data and a statistical decay mechanism should be carefully applied to realistic problem. For example, the charged particle emission channels are treated as an evaporation process from a compound nucleus. This is only valid if induced neutron

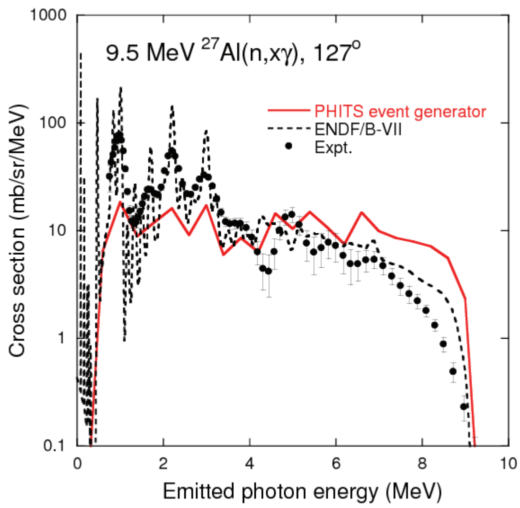

Fig. 7 Double differential cross section for the ^{27}Al(n,xγ) reaction at 127°. Experimental data were taken from Reference 8.

energy is less than 10 MeV. Above 10 MeV the main process will be a preequilibrium emission, which removes more energy than the evaporation, consequently the excitation energy of the residual nucleus will be lower. In future, a more realistic physical model should be adopted.

IV. E-Mode Calculation Examples

By E-mode in PHITS for low energy neutron transport phenomena, we can calculate many new quantities which cannot be obtained by using only the evaluated nuclear data, e.g. kinetic energy distribution of charged particles, two-particle correlation, and so on. Here we show an example of the event generator mode in PHITS, i.e. energy distribution from the ^{10}B(*n*, α)^{7}Li and ^{6}Li(*n*, α)*t* reactions, which is a typical quantity beyond one-body observable. The thermal neutron induced ^{10}B(*n*, α)^{7}Li reaction will be very important in the microdosimetric analysis for the boron-neutron capture therapy (BNCT). The ^{6}Li(*n*, α)*t* reaction is also important in the analysis for the response of neutron detectors. In these reactions, the total reaction cross section

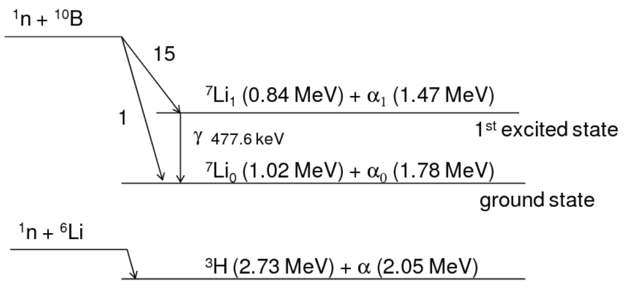

Fig. 8 Flowchart of the n+^{10}B and n+^{6}Li reactions

and branching the reactions are taken from the nuclear data library, energies of emitted particles are calculated by the special statistical decay model with isotropic angular distribution in the CM system. **Figure 8** shows a flowchart of the ^{10}B(n, α)^{7}Li and ^{6}Li(n, α)t reactions.

In the thermal ^{10}B(n, α)^{7}Li reaction, after the capture of thermal neutron by ^{10}B, ^{11}B compound nucleus is formed in the intermediate state. The primary decay mode for this system is alpha particle decay. For the decay, the residual lithium nucleus can be left in either its ground state ^{7}Li or in its first excited state ^{7}Li* which decays by prompt gamma emission with E_{gamma} = 477.6 keV. In the first case, the alpha particle has the kinetic energy T(α_0) = 1.78 MeV, we call this 'alpha zero' α_0 and in the second case, T(α_1) = 1.47 MeV, called 'alpha one' α_1. In E-mode, the branching ratio ^{10}B(n, α_1)/^{10}B(n, α_0) was set to be 15 taken from experimental data.[9)]

For the ^{6}Li(n, α)t reaction, the most decay mode is alpha decay system and tritium can be left in the ground state. The alpha and tritium particles have the kinetic energy T(α) = 2.05 MeV and T(t) = 2.73 MeV, respectively.

E-mode in PHITS includes these specific reactions and traces all correlations of ejectiles keeping the energy and momentum conservation in a collision. As mentioned earlier, the cross sections for charged particles are produced by the special statistical decay model while evaluated nuclear data is used only for the total cross section and branching the reactions. **Figures 9** and **10** shows calculated energy distributions of produced particles for the thermal ^{10}B(n, α)^{7}Li and 24 keV ^{6}Li(n, α)t reactions and comparisons to experimental data[9)] which was presented in arbitrary unit.

The distortion of peaks in calculations is resulted from the target thickness. The experimental data includes not only the contribution of the target thickness but also the energy resolution and the wall effect of a detector. In general, the shape of calculated energy distributions and the ratio of each charged particle agree quite well with experimental data. These examples indicate that the energy distribution of charged particles and residual nuclei can be described by E-mode in PHITS even for low energy neutron induced reactions without additional evaluated nuclear data. In addition to these inclusive observables, the correlation of these emitted charged particles and residual nuclei are well described in event-by-event. So E-mode would be applied to the calculation of the distribution of energy deposition in a cell, the microdosimetric analysis of the biological effects

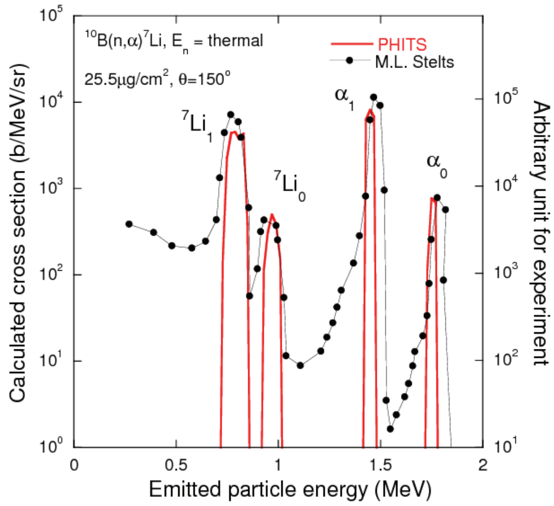

Fig. 9 Calculated energy distributions of produced particles for the thermal ^{10}B(n,α)^{7}Li and comparisons to experimental data. Experimental data were taken from Reference 9.

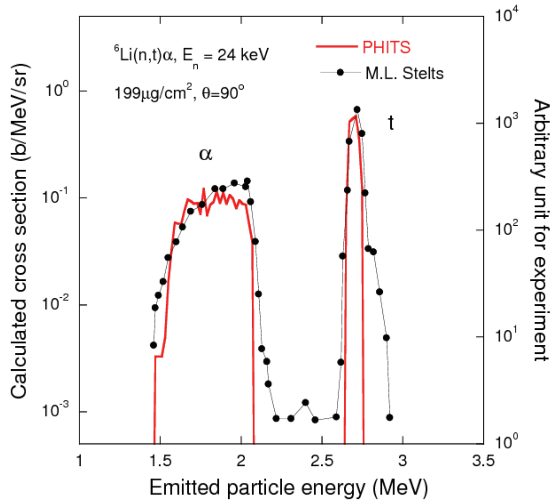

Fig. 10 Calculated energy distributions of produced particles for the thermal ^{6}Li(n,t) α and comparisons to experimental data. Experimental data were taken from Reference 9.

and many other correlated quantities.

V. Summary

The E-mode in PHITS has been developed to reconstruct an event with the energy and momentum conservation for the low energy neutron transport phenomena. To investigate the validation of the E-mode in the energy region below 20 MeV, the activation cross section and the double differential cross sections of charged particles and photons were calculated and compared with the evaluated nuclear data and experimental data. As results, calculated results reproduced the data very well, As applications of E-mode, we indicated new calculations about the energy distributions of charged particles for the thermal ^{10}B(n, α)^{7}Li and 24 keV ^{6}Li(n, α)t reactions. These reactions are important in the microdosimetric analysis for BNCT and the response of neutron detectors. The shape of calculated energy distributions and the ratio of each charged particle agree well with experimental data. At the present, there are some problems in E-mode. For an example, in higher energy region above 10 MeV, we should take into account the other reaction mechanism such as preequilibrium emissions and break up processes instead of the statistical decay model in the present E-mode model. However, E-mode of PHITS may have a great ability to analyze the microdosimetric biological effects, the single setup error of semiconductor, and to many other fields which are related to the correlated quantities beyond one-body observables.

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