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Estimation of double-differential cross-sections of ^{9}Be(p,xn) reaction for new nuclear data library JENDL-5

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Abstract. Double-differential cross-sections of the ^{9}Be(p,xn) reaction are newly evaluated based on the Wakabayashi's function and neutronics analysis up to 12 MeV for a new nuclear data library, JENDL-5. We devoted our efforts especially to the re-optimization of the absolute cross-sections and the interpolation of the neutron energy spectra. Through the comparisons between the thick target yield measurements and Monte-Carlo simulations at different proton energies and neutron emission angles, we conclude that JENDL-5 gives the best evaluation in the world.

Keywords: Nuclear data, ^{9}Be(p,xn) reaction, Double-differential cross-section, Wakabayashi's function, Interpolation, Neutronics simulation, Thick target yield, JENDL-5

1. Introduction

The cross-section of the ^{9}Be(p,xn) reaction is highly important for the design of neutron sources with small accelerators. However, its evaluated values in the world's nuclear data libraries have large uncertainties since available experimental data-sets of the cross-sections are very scarce, and some data does not match each other. It is also because the study of the nuclear theories/modelings, which is often applied to the prediction of cross-sections or interpolation of experimental values, is still on a scientific challenge for the few-body systems, viz., light nuclei such as ^{9}Be.

Looking at the status of absolute cross-section measurements which are available in the experimental database EXFOR [15], several data-sets are certainly found below ∼15 MeV. However, most of them were measured before the 70s, in which the data are given in a narrow energy region and discrepant each other by more than 20%. Among the existing data, the experimental data of Bair *et al.* [2] gives the excitation function in a relatively wider energy range (4–14 MeV) than the others, but the measurement is a so-called relative one which means the absolute information is totally absent. According to the EXFOR database, there are similar situations also for the measured differential cross-sections.

In the nuclear data evaluation, the statistical theory [8] which is combined with nuclear structure models is often used for the interpolation of available experimental data. It is also applied to the prediction/estimation of

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differential and double-differential cross-sections (DDX). Indeed, our nuclear reaction model code CCONE [12] is known as one of the powerful tools for the nuclear data evaluation, with a minimal optimization of the model parameters therein, as it has been applied to the development of our nuclear data libraries, e.g., JENDL-4.0 [17]. However, it is difficult to apply such a kind of code to the light nuclei ($A \lesssim 20$) because they are few-body systems which may be out of the scope of the statistical theory. Also, understanding/modelling the structure of light nuclei is at the stage of a scientific study.

One of our special purpose nuclear data libraries, JENDL-4.0/HE [13], provides the evaluated cross-sections data up to 200 MeV to be used for the design of accelerator-based applications such as the neutron sources, accelerator-driven system for the transmutation of radioactive wastes, and so forth. Indeed, this library is implemented in the Particle and Heavy Ion Transport Code System (PHITS) code [16] for an optional use. This library certainly includes data of ^{9}Be for incident protons, but we managed to apply the CCONE code to the data evaluation for ^{9}Be despite the inaccuracy of the measurements and nuclear models mentioned above, which means the data for p+^{9}Be in JENDL-4.0/HE could have a large uncertainty. Quite recently, one of the authors, Wakabayashi *et al.* [21], proposed a function which describes the cross section and DDX of ^{9}Be(p,xn) where a number of parameters are optimized with selected experimental data-sets. The function is expected to be more suitable to the practical nuclear data evaluation since it is more flexible than the nuclear models.

The objectives of the present study are:

- evaluation of the cross section for the ^{9}Be(p,xn) reaction based on the Wakabayashi's function,
- generation of DDX with a physically reasonable interpolation scheme for the ^{9}Be(p,xn) reaction based on the function

for our new nuclear data library JENDL-5 [11] which intends to provide evaluated nuclear data not only for the nuclear energy but also for the accelerator-based applications.

2. Data evaluation for ^{9}Be(p,xn)

2.1. The Wakabayashi's function

The energy dependence of the absolute cross-section is rather smooth except for the lower energy region ($E_n \lesssim$ 5 MeV) where several resonances are observed in the available measurements. The neutron energy spectrum from the ^{9}Be(p,xn) reaction is characterized by a continuum part and peaks which correspond with the transition to the ground and low-lying excited states of the residual nuclei ^{9}B$^{(\star)}$. These characters are so complicated that it is difficult to predict them consistently only by a combination of nuclear models. Recently, one of the authors, Wakabayashi *et al.* [21], proposed a function which was designed to describe all the characters up to $E_n = 12$ MeV, in which the parameters therein were optimized by selected experimental data-sets. According to the neutronics analysis with GEANT-4 [1], the function gives a reasonable estimation of thick target yield (TTY) better than those with existing nuclear data libraries. Unfortunately, MCNP [22] or PHITS [16] cannot use the function directly since they are designed to use nuclear data libraries or built-in models (e.g., Ref [4]) for high-energy nuclear reactions.

2.2. Incorporation of the function to nuclear data file

In the present study, we incorporated the Wakabayashi's function to a nuclear data file, which finally enables us to perform neutronics analyses with both MCNP and PHITS. In a first step, the energy dependent cross-section of the ^{9}Be(p,xn) reaction was calculated with the function, taking care of the selection of the energy grids to fully describe the resonant shape in the lower energy region. In the next step, we produced data table of the neutron energy spectra from the function at different proton energies and emission angles. In this case, much attention was paid also to the determination of neutron energy nodes especially around the peak positions to minimize the data

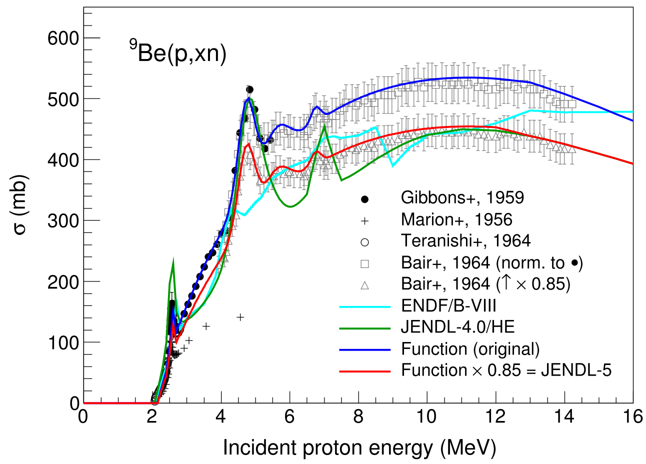

Fig. 1. Evaluated and measured cross-sections of the ^{9}Be(p,xn) reaction.

size. Such point-wise data-sets were compiled in the ENDF-6 format [20] file.[1] Since a normalized angle-energy distribution was required to be compiled for each incident energy in the ENDF-6 format, we normalized DDX with respect to the neutron energy E_n and emission cosine angle μ for each proton energy E_p as,

$$\int dE_n \int d\mu f(\mu, E_p, E_n) = 1 \tag{1}$$

where $f(\mu, E_p, E_n)$ is the normalized DDX to be given in the data file.

In compilation process, an interpolation scheme must be given to the data-tables because the data we generated from the function were forced to be discretized in principle. In the present study, the linear-linear interpolation was assumed for excitation function and also for each neutron energy spectrum at an emission angle. On the other hand, the two-dimensional unit-base [20] was assumed for the interpolation between the neutron spectra of two adjacent incident proton energies to minimize pile-ups of peaks which appear if the normal one-dimensional interpolation is used. Finally, we replaced the ^{9}Be(p,xn) data in JENDL-4.0/HE with the present data tables from the threshold energy of the reaction to 12 MeV. Such a data merging is necessary because a complete data set of cross-sections (which includes those for the other types of reactions) is expected in the neutronics simulation.

Figure 1 shows the cross-section obtained from the function together with available experimental data [2,7,19] and evaluations. It is clear that the original function is designed to reproduce the measured data by Gibbons *et al.* [7] and the normalized data by Bair *et al.* [2]. Figure 2 illustrates an example of DDX extracted from the present data file with experimental data [3]. The two peaks observed in this spectrum correspond to the ground and excited states of ^{9}B, with a full width at half maximum of 0.07 MeV [21]. As shown by one of the curves (INT = 2), it is difficult to produce sharp peaks correctly if we use the normal linear-linear interpolation. This issue encountered with the numerical data-table is solved in the present study with the unit-base interpolation, where we kept the ratio of the peak energy to maximum energy constant in the unit base, for the neutron spectrum interpolation as illustrated by the other curve (INT = 22). It is concluded that the function gives a reasonable estimation of the cross-section and DDX, and the applied interpolation schemes are reasonable.

2.3. Neutronics analysis

Although the measured cross-sections including DDX are very scarce, there exists experimental data of TTY which were published in the current century, at different incident energies and emission angles, fortunately. Therefore, those measurements are quite useful to validate the present nuclear data file generated as described above. For

[1] We adopted the laboratory angle-energy law (MF = 6, LAW = 7) in the ENDF-6 format to compile the normalized spectra.

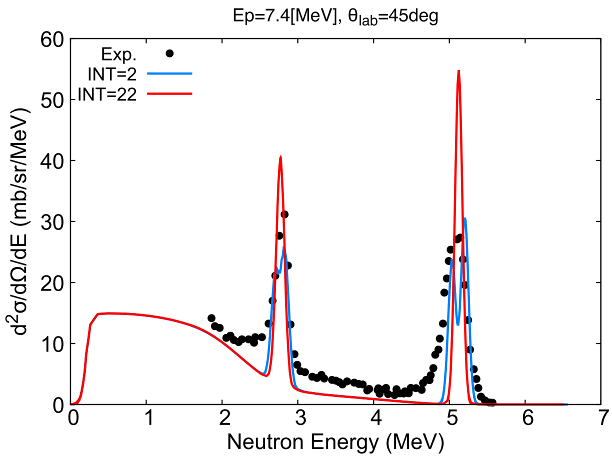

Fig. 2. Example of DDXs which are extracted from the present data file with the interpolation. The red curve (INT = 22) shows data with the unit-base interpolation while the blue curve (INT = 2) shows data with the normal linear-linear interpolation. Note that those curves are taken from the final data file (JENDL-5) where the absolute cross section is reduced by 15% from the original function.

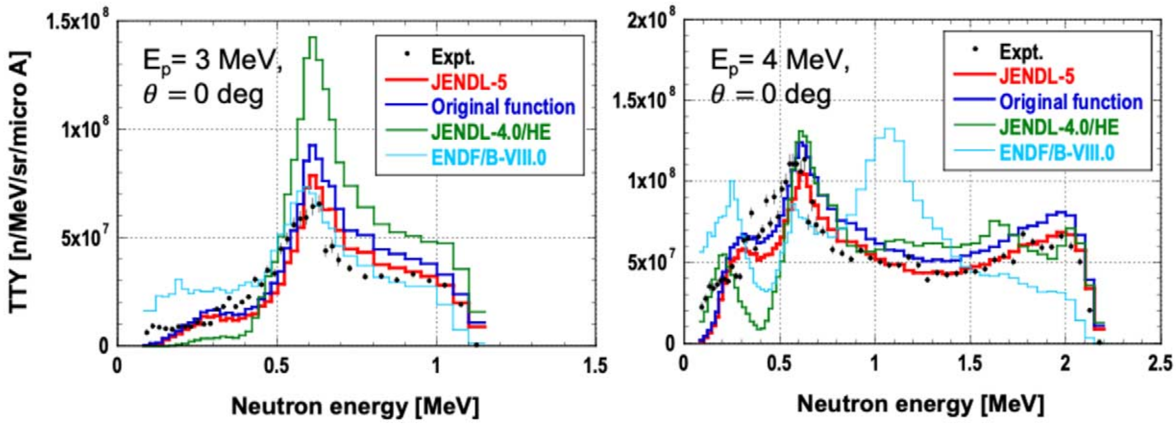

Fig. 3. Example of simulation results for the thick target yield for E_p = 3 and 4 MeV at emission angle of 0 deg.

example, the measured data by Howard *et al.* [9] are quite useful as they give neutron energy spectra at $E_p = 4, 5$ and 6 MeV from the most forward to backward emission angles. Before carrying out the neutronics analysis, the ACE format [6] file was generated for the Monte-Carlo simulation. We used the NJOY2016 code [14], which was modified for JENDL-5, for the data processing. Note that the two-dimensional unit-base interpolation was dealt as the linear-linear interpolation because it was not supported in NJOY and Monte-Carlo codes, unfortunately.

Neutronics simulations were performed by the MCNP code [22] with the ACE files of the present data file (original function), JENDL-4.0/HE [13] and ENDF/B-VIII.0 [5]. Figure 3 illustrates an example of the TTY simulation results together with the experimental data by Howard *et. al.* [9]. The result obtained with ENDF/B-VIII.0 is not consistent with the shape of the measured data. That with JENDL-4.0/HE seems to give a better estimation, but it largely underestimates the experimental data in the lower energy region. It is obvious that the result (original function) with the present file based on the original Wakabayashi's function simulates the measured neutron spectrum better than the existing libraries. However, the result with the present data overestimates the measured spectrum by $10 \sim 20\%$. Such a discrepancy is also systematically confirmed in other proton energies and emission angles.

2.4. Estimation of cross-sections for JENDL-5

Even though we have confirmed that the function already gave the best estimation of TTY among the data libraries in the world, we noticed that the present data overestimated measured TTY systematically by $10 \sim 20\%$. As we already mentioned above, the measured data-sets of the absolute cross-sections do not match each other. Besides, the experimental excitation function by Bair *et. al.* is a relative measurement, which means the absolute value was not known. Therefore, the present cross-section should also have a uncertainty of the same order, which may result in a systematic overestimation of the measured TTY.

For the new nuclear data library JENDL-5, we finally decided to reduce the absolute cross-section by 15% from the original function as illustrated in Fig. 1. Figure 3 demonstrates that the prediction ability of the neutronics simulation with the re-optimized data file (JENDL-5) is much better than that based on the original function. From similar comparisons at other proton energies and neutron emission angles, we conclude that the present data file (JENDL-5) gives the best estimation worldwide.

2.5. JENDL-5 and remarks on unsolved issue of $p + {}^{9}\mathrm{Be}$ evaluation

The new nuclear data library JENDL-5, which was compiled in the ENDF-6 format, was released in December 2021.[2] This is the first major update of the previous version JENDL-4.0 which dates from 2010. The features of JENDL-5 relevant to the small accelerator might be summarised as follows:

- revision of a large part of JENDL-4.0 such as neutron reaction data, thermal scattering law data
- neutron activation cross section data
- the first originally evaluated thermal scattering law data for 16 materials such as light and heavy water, benzene, and ethanol
- reaction data induced by light charged particles (proton, deuteron and alpha-particle) and photon.

The evaluation for ^{9}Be is included in the proton-induced sub-library where the present data are compiled up to 12 MeV. Above 12 MeV, the data are taken from JENDL-4.0/HE, where a discontinuity of the ^{9}Be(p,xn) reaction cross section at the boundary energy does not appear between JENDL-5 and JENDL-4.0/HE as illustrated in Fig. 1. This is probably not a coincidence because the characteristics of nucleus tend to fade out as an excitation energy of compound nuclei (incident proton energy) becomes higher.

JENDL-5 application libraries including ACE format files will also be soon available. Touching upon the PHITS code, the current version of code package includes JENDL-4.0 in the ACE format. Similarly, JENDL-4.0/HE is also included for a number of nuclei relevant with accelerator applications. In the future, instead of JENDL-4 and JENDL-4/HE, JENDL-5 for neutrons below 20 MeV and for neutrons and protons up to 200 MeV for specific nuclides will be bundled to the PHITS package.

Although we have obtained the nuclear data evaluation for $p + {}^{9}\mathrm{Be}$ which gives the best estimation of the neutron spectra in the world, there still exists an issue to be solved in the future. Indeed, we always observed overestimations of the measured TTY of Howard *et al.* at backward angles as illustrated in Fig. 4. The other libraries also give shapes which are different from the experimental data. There should be a fundamental issue on description for the angular distribution both in the Wakabayashi's function and nuclear models used in the previous libraries. In near future, we plan to update the function with incorporation of the coupled-channel theory [18] only for the direct reaction to overcome such a remaining issue. Also, it may be meaningful to look into a recent progress on the machine-learning approach to the data evaluation [10].

[2] https://wwwndc.jaea.go.jp/jendl/j5/j5.html

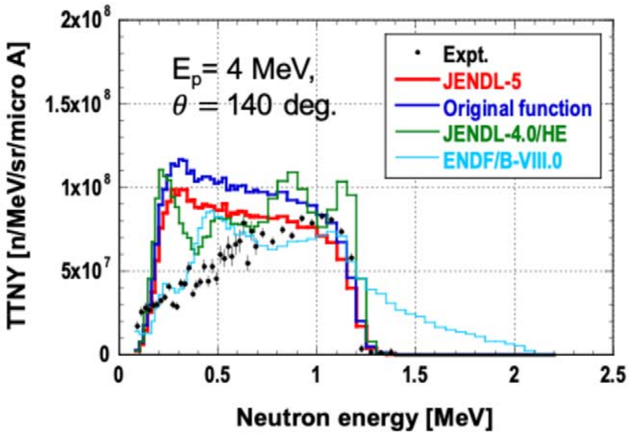

Fig. 4. Example of simulation results for the thick target yield at the backward angle.

3. Conclusion

We have evaluated the cross section and DDX of the ^{9}Be(p,xn) reaction based on the function proposed by Wakabayashi *et. al.* up to 12 MeV. Through the neutronics analysis, we finally decided to reduce the absolute cross-section by 15% from the original one to provide a better agreement with the TTY measurements. The evaluated cross section and DDX data are compiled in the ENDF-6 format with physically reasonable interpolation schemes. This data is merged in our new nuclear data library JENDL-5 released last December. We conclude that JENDL-5 gives the best prediction worldwide of neutron spectra from a beryllium target bombarded with proton.

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