Monte-Carlo simulation of transmutation based on experimental nuclear data

S. Ebata,^{*1} D. Ichinkhorloo,^{*1} and M. Aikawa^{*1,*2}

The management of long-lived fission products (LLFPs) in nuclear reactors is one of the most important tasks in nuclear engineering. The transmutation of LLFPs is a promising technology to reduce and reuse high-level radioactive nuclear wastes. Reaction cross sections of the transmutation are fundamental and essential information in nuclear applications. The cross sections of proton- and deuteron-induced reactions on the LLFPs $^{93}\mathrm{Zr}$ and $^{107}\mathrm{Pd}$ were measured using the inverse kinematics technique in RIBF.^{1,2)}

Furthermore, macroscopic simulations based on a realistic condition are essential for the feasibility study of the transmutation. A Monte-Carlo simulation code PHITS³⁾ is adopted and used to design the nuclear applications for the transmutation of LLFPs in our project. However the transmutation reaction cross sections calculated using PHITS are partially different from the experiment data.^{1,2)} To avoid the discrepancies, we need to induce the recent experimental data directly in simulations. A function named Frag Data is implemented in PHITS to use external cross section data. By using this function, we can reflect the experimental data in the macroscopic simulations.

The Frag Data function requires an external data file of cross sections for each reaction system consisting of a target and projectile. The file includes the total, production and double differential cross sections of each outgoing particle for several incident energies. The production cross sections of heavy residual nuclei in a target could be obtained in previous experiments.^{1,2)} The double differential cross sections of secondary light particles (neutron, proton, deuteron and ⁴He) are also required because the data are expected to have large effects on the transmutation. The cross sections of such light particles, however, were not measured in the experiments. Therefore, we adopt results for the secondary particles calculated using the default PHITS simulation as inputs of the file.

For the simulation of the proton-induced reaction, the process to prepare the Frag Data input files is as follows. First, simulations for 100- and 200-MeV proton-induced reactions on thin ¹⁰⁷Pd and ⁹³Zr targets (5 μ m thickness) were performed with the trial number set to 10⁶. From the simulations, the double differential cross sections of the secondary light particles were obtained and inserted into the file. Next, the experimental data, *e.g.* production cross section of the residual nuclei (49 isotopes from Ag to Mo for ¹⁰⁷Pd and 44 from Nb to Br for ⁹³Zr), were inserted. After the preparation of the Frag Data file, we can perform PHITS simulations of a more realistic situation based on the experimental data.

A simulation using the Frag Data function for proton-induced reactions on a thin ¹⁰⁷Pd target was performed for confirmation. The simulation result of production cross sections of Ag isotopes (open squares) is shown in Fig. 1, which is compared with the experimental data (filled squares) and the result without the Frag Data function (filled circles). We can confirm that the result with the Frag Data function reproduces the same result as the experiments.



Fig. 1. Production cross sections of Ag isotopes in the $^{107}Pd+p$ reaction at 200 MeV.

The Frag Data function in PHITS can directly import bare experimental data of cross sections to simulations. We performed simulations of transmutation with the function and then confirmed the reproduction of experimental cross sections. Based on the Frag Data files, we can perform macroscopic simulations with realistic conditions for the feasibility study of transmutation.

This work was funded by the ImPACT Program of the Council for Science, Technology and Innovation (Cabinet Office, Government of Japan).

References

- H. Wang *et al.*, Prog. Theor. Exp. Phys. **2017**, 021D01 (2017).
- S. Kawase *et al.*, Prog. Theor. Exp. Phys. **2017**, 093D03 (2017).
- 3) T. Sato et al., J. Nucl. Sci. Technol. 50, 913 (2013).

^{*1} Faculty of Science, Hokkaido University

^{*&}lt;sup>2</sup> RIKEN Nishina Center