MCNP simulation of neutron spectrum modification by aqueous Gd sample in prompt gamma activation analysis

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1. Introduction

The k_0-standardization has been applied to SNU-KAERI prompt gamma activation analysis (PGAA) facility [1]. For the determination of the prompt k_0-factor, γ-rays from a comparator and an analyte are measured during the neutron irradiation. To analyze ^{155}Gd and ^{157}Gd, Cl was used as a comparator. ^{157}Gd is a strong neutron absorber ($\sigma_{capture}$ at 0.025 eV is 254996 b [2]), and its prompt γ-rays (up to 6750.05 keV) forms high Compton continuum in the γ-ray spectrum which obstructs resolving the 1951.14 keV peak from the ^{35}Cl(n,γ) reaction. To obtain an appropriate count rate for the 1951.14 keV peak relative to those of prompt γ-ray peaks of Gd, the standard Gd solution (10,014 ppm in 0.97%wt HNO_3) was diluted by adding purified water. In this case, neutron scattering with H and O in water causes the distortion of the incident neutron spectrum. To investigate the effect of neutron scattering and obtain the effective neutron spectrum within the sample, MCNP Monte Carlo simulations are carried out in this study.

2. Method and results

The geometry for MCNP simulations is shown in Fig. 1. The Gd sample is irradiated with the neutron beam at the incident angle of 45°. The incident neutron beam is approximated to a parallel beam with a uniform spatial distribution. The sample consists of 0.107 ml of water and 5.7 mg of Cl. Na and N are ignored in simulation because their macroscopic cross sections are much smaller than that of Gd. The incident neutron spectrum is shown in Fig. 2, which has been refined in the previous studies [3]. Unlike other diffracted beam encountered in neutron scattering facilities, the diffraction orders two to five mostly contribute to the incident flux. Either this spectrum or a simplified spectrum is coded into the MCNP input card.

MCNP5 code is used with cross-section data from the ENDF/B-VI library [4] including thermal S(α,β) table.

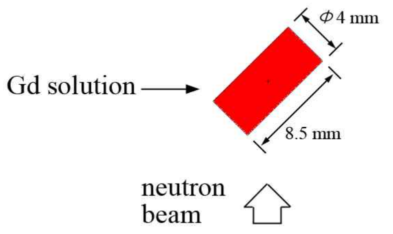

Fig. 1. Geometry of MCNP calculation.

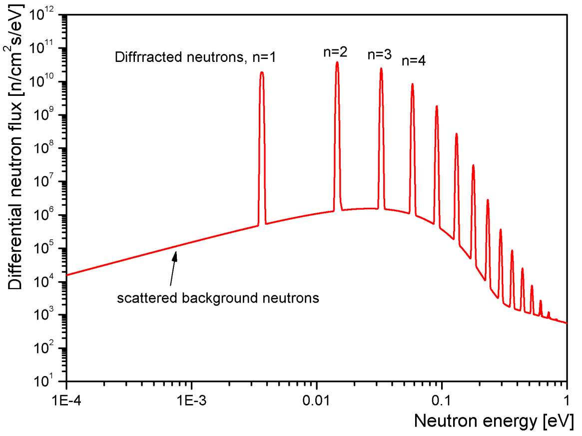

Fig. 3. Incident neutron flux spectrum in the SNU-KAERI PGAA facility.

The track length estimate tally, F4 is used for the predicting the neutron flux spectrum averaged over the sample volume. The number of neutron histories is 10^{10}.

To compare spectrum distortions between different diffraction modes, the diffracted spectrum of each order was used as MCNP input spectrum. The neutron flux spectrum calculated for the second diffraction order (0.0327 keV) is shown in Fig. 3. It is obvious that 45% of incident neutrons are scattered with and captured by H, O and Cl. The peaks on the continuum are produced by inelastic scattering with H, which can be described by thermal S(α,β) scattering models [5].

The simulation for the whole neutron spectrum as an incident spectrum is performed next. The neutron spectrum averaged over the sample volume is shown in Fig. 4. In this case, 37% out of the main diffracted neutron were scattered and absorbed.

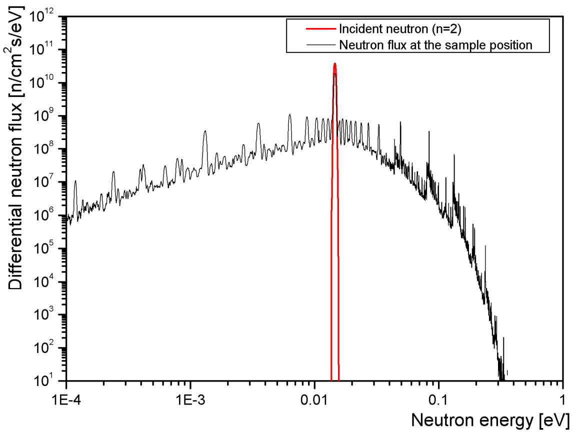

Fig. 3. Calculated neutron flux spectrum at the sample position (incident neutron flux: single energy neutron, n=2).

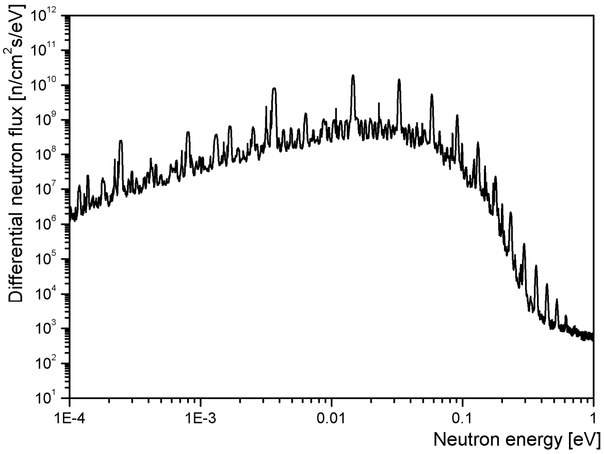

Fig. 4. Calculated neutron flux spectrum at the sample position (incident neutron flux: whole spectrum).

3. Conclusion and further work

37% out of the main diffracted neutron were scattered with the elements of sample solution, which led to the rising of the continuum part in the neutron spectrum. As this spectral distortion effect has been neglected in k_0-standardization to date, the effect needs to be investigated in detail for calculations of effective g-factors and k_0-factors of ^{155}Gd and ^{157}Gd.

Acknowledgement

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