Analysis of Doppler-broadened peak in thermal neutron induced $^{10}B(n,\alpha\gamma)^{7}Li$ reaction by using HyperGam

H.D. Choi, N.S. Jung and B.G. Park
Seoul National University, Shinlim-Dong, Gwanak-Gu, Seoul 151-744, Korea
vandegra@plaza.snu.ac.kr

1. Introduction

The line shape functions for the Doppler-broadened (DB) γ-ray spectrum are reviewed in the $^{10}B(n,\alpha\gamma)^{7}Li$ reaction occurring in a surrounding medium where the excited ^{7}Li nucleus is slowed down and stopped before decay. Convolution with the detailed response of a germanium detector is achieved in an analytic form by taking into consideration the simplest case of electronic stopping. A numerical study for the analysis of ^{10}B by thermal neutron capture is conducted by performing a parametric search and fitting the measured spectrum in a least-squares approach. In comparison with the previous numerical approach using the same analysis, the computational speed is increased and reliable information concerning the stopping power of the medium is obtained with the uncertainty estimation. Implementation of the routine analysis of ^{10}B is facilitated on a recent version of the γ-ray spectrum analysis package HyperGam.

2. Analysis of measured γ-line shapes in the $^{10}B(n,\alpha\gamma)^{7}Li$ reaction

If the initial recoil velocity of the excited nucleus is not high and practically all of the excited nuclei decay out before reaching the low velocity region where nuclear stopping dominates, the mechanism of stopping is simply restricted to the electronic collisions. Here, the line shape with no consideration of the angular correlation is given, as [1,2,3]

$$\frac{dn(\varepsilon)}{d\varepsilon} = \begin{cases} \frac{N_0}{2}\frac{\lambda/D}{(\lambda/D)-1}\left\{1-\left|\varepsilon\right|^{(\lambda/D)-1}\right\}, & \lambda/D \neq 1, \\ \frac{N_0}{2}\log\frac{1}{\left|\varepsilon\right|}, & \lambda/D = 1, \end{cases} \quad (1)$$

where N_0 is the total number of γ-ray emission, λ is the decay constant of the excited nuclear state, D is the degradation constant and ε is defined as $\varepsilon \equiv (E_\gamma - E_0)c/E_0 v_0$. Here, E_γ is the Doppler shifted energy of γ-ray, E_0 is the energy emitted from a stationary nucleus and v_0 is the initial velocity of the recoil nucleus.

The line shape in Eq. (1) is dependent on the sample medium in terms of degradation constant D. In addition, there could be γ-rays of energy near 478 keV in the DB peak in the case of $^{10}B(n,\alpha\gamma)^{7}Li$ reaction with interfering lines originating from impurities of other component elements in the sample. Therefore, multi-parameter peak fitting is performed to resolve the overlapping peaks from the DB peak and to describe the DB peak by the degradation constant D. In the fitting process, a convolution of the emission spectrum with the detector response function is performed in a convergent series thereby reducing the computational time required for multi-parameter peak fitting in a routine analysis task. The main part of germanium detector response is described by a Gaussian function and the response functions used for the low-energy tail and the step-background are taken from the HYPERMET code [4]. The details of developed formulae and numerical implementations are described in a recent paper [5].

To check the numerical accuracy and speed of the developed formulae, a calculation of the convolution integrals is done by numerical integration using the Gaussian quadrature routine 'quadl' in MATLAB. Using the formulae developed in this study with the convergence criteria of 10^{-6} and using the technique of vectorizing variables, the calculation speed was observed to increase by a factor of approximately 2 compared to that of numerical convolution at the same accuracy. For the case of a short-term tail convolution, the speed was lower due to multiple sums in the obtained formula. Hence, numerical integration is adopted for the convolution of the short-term tail function. Within the adopted numerical accuracy (10^{-6}), both routines give identical results.

3. Analysis of DB peak in the $^{10}B(n,\alpha\gamma)^{7}Li$ reaction

In Figure 1, the result of an example analysis is shown for the DB peak that is emitted from the $^{10}B(n,\alpha\gamma)^{7}Li$ reaction induced by thermal neutron. The sample is boric acid (H_3BO_3) prepared by drying a diluted aqueous solution. For peak fitting, the Gaussian width parameter is fixed by considering the shape-energy dependency obtained from analyzing the neighboring single energy peaks. The maximum DB width of the emitted spectrum is also fixed to the physical value of 7.6 keV with a scale conversion into the channel unit. Hence, parameters are searched for the center and height of the DB peak, degradation parameter $\alpha \equiv \lambda/D-1$, the heights of the low-energy tail and step-background, and the continuous

linear background including those for the interfering Gaussian peaks. The heights of the low-energy tail and step-background determined in the fit are very small in this measurement: 1×10^{-3}. The background peaks around the 552, 556, 558 and 568 channels are trivial for obtaining the D-value but improve the fit. The final reduced χ^2 is 1.3. The required time to obtain this result is approximately two minutes. In Table 1, the obtained value of degradation constant D is compared with other reference values which are based on either theories or experiments. The D-value of the SRIM calculation is obtained by fitting a line to the numerical stopping power in the energy region of 90–600 keV [6]. Definite inconsistency is seen between different literature values by considering the associated uncertainties. There are differences in the analysis methods, detector response functions and target material conditions in these experimental works [7,8]. There are also interesting studies to claim the chemical binding effect in the stopping power of compounds, suggesting a deviation from Bragg's rule. Therefore, a more detailed discussion of this topic requires further research. Other example of the multi-parameter peak fitting is the decomposition of the DB boron peak and a strongly interfering γ-ray peak (472 keV) emitted from ^{23}Na capturing neutrons. The target sample is spinach reference material (SRM 1570a) [9]. The same measured spectrum reported in an earlier study [10] is re-analyzed by the current algorithm developed in this study. The new fit resulted in a D-value of 1.56±0.08 ps^{-1} and a boron concentration of 37.3±1.1 μg/g. The results for the boron concentration of spinach sample are summarized in Table 2 for comparison with

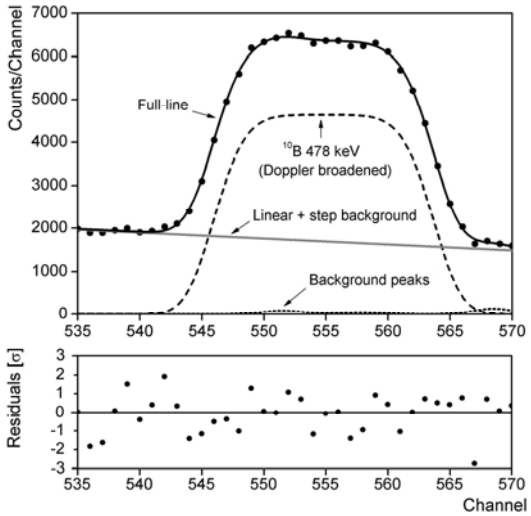

Fig. 1. Analysis of DB spectrum for boric acid (H_3BO_3, B mass 17.6 μg). The short tail and step-background parts are vanishingly small but are included in the plot. The determined values are a DB peak area I of 80,300 ± 760 and a degradation parameter α of 7.16 ± 0.21.

Table 1. The degradation constants D (ps^{-1}) obtained by various works on the slowing down of a ^{7}Li ion in boric acid (polycrystalline H_3BO_3, density 1.435 g/cm^3)

Theoretcal		Experimental		
LSS theory	SRIM [6]	Sakai *et al*. [7]	Szentmiklósi *et al*. [8]	This work
1.50 [7]	1.34	1.48	1.29 ± 0.01	1.17 ± 0.03

Table 2. Comparison of the boron concentration of a spinach sample with the values of a previous work and a certified value

Sample	Mass [mg]	Analyzed boron peak count rate [cps]	Boron concentration [μg/g]		
			This work	Previous work [10]	Certified [9]
SRM 1570a spinach	113.2 ± 0.1	9.64 ± 0.27	37.3 ± 1.1	35.2 ± 1.0	37.6 ± 1.0

the value of the previous analysis and a certified value. Closer agreement with the certified value was observed in the present analysis.

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