Modeling of Detector Response Function in Neutron Depth Profiling

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1. Introduction

A Cold Neutron-Neutron Depth Profiling (CN-NDP) system has been designed and developed at HANARO, a 30 MW research reactor at the Korea Atomic Energy Research Institute (KAERI). In the previous study [1], basic theory for analysis of NDP spectrum was discussed and the analysis code for the ideal case (without energy broadening effect) NDP spectrum was developed. In the real case, the depth profiles derived directly from measured NDP spectrum deviate from the true ones. The differences are caused by the energy resolution ΔE of the system which is composed of several contributions. The main contributions to the energy broadening are the detector energy resolution, geometrical acceptance angle, energy loss straggling and multiple scattering of the charged particles. In this study, the amount of the energy broadening of the NDP spectrum is determined, and the predicted spectrum is modeled as a Gaussian process based on the detector response function.

2. Contributions to the energy broadening of the NDP spectrum

The NDP spectrum acquired by the spectrometer is a convolution of the actual energy distribution of the charged particles and the measurement system. Each component of the system, i.e. the sample, geometry, detector and the measurement electronics, has its own energy uncertainties, hence causes spectral broadening to the measure energy of the charged particle. Each broadening mechanism can be treated independently [2].

Main interactions in the sample substrate that cause the energy uncertainties are energy loss straggling and multiple small-angle scattering. The energy loss straggling is caused from the statistical nature of the slowing down process. When the charged particle is emitted at certain energy, the actual energy loss deviates owing to the stochastic process of nuclear and electronic interactions with the host nuclei and electrons. The simplest approach to determine the energy broadening by the energy loss straggling is the Bohr model [3]. There are numerous small-angle scatters that cause charged particles to travel slightly different distances in the sample before escaping the surface, thereby causing variations of particle path length. The multiple small- angle scattering is predominantly due to the nuclear collisions.

Geometric uncertainties arise from the finite size of the detector and sample. Since the detector subtends a finite acceptance angle, a range of emittance angles exists for a given emission depth. Variation in path lengths results in spread of measured energies.

Energy broadening from the detector and measurement electronics are caused by the stochastic nature of ion reactions in the detector material and the electronic noise of the system. This effect originates from the inherent detector energy resolution, electronic noise of the amplifier & data acquisition chain and the system noise from the vacuum pump and etc.

The standard deviation of the energy broadening effects for 1472 keV alpha particle from ${}^{10}B(n,\alpha)^7Li$ reaction is shown in Fig. 1 as a function of depth. The energy broadening due to the straggling($\sigma_{\text{straggling}}$) and multiple scattering($\sigma_{\text{scattering}}$) were obtained from the Bohr model and TRIM calculation [4] for alpha particles born at different depths in silicon. And the detector resolution(σ_{det}) of the CN-NDP system was determined experimentally to be 26 keV from the measurement for the SRM-93a sample. The amount of the energy broadening by the detector energy resolution was assumed a constant for the whole depth in the sample. The geometrical effect was not included in this calculation, since its contribution is small in the usual NDP measuring geometry with the particle detector situated in the direction of the sample surface normal or nearby. Total energy broadening was the quadrature sum of the each contribution.

3. Detector response function and modeling for the NDP spectrum

The relation between the number of counts recorded in bin *i* of the MCA energy spectrum (bin width 2Δ and midpoint energy E_i) and the depth profile $C(x)$ at the depth *x* can be expressed as

$$
y_i = \int_0^{x_{\text{max}}} C(x) R_i(x) dx
$$
 $i = 1, ..., N$

where the detector response function $R_i(x)$ which gives the probability that a particle created at the depth *x* will

Fig. 1. Energy broadening due to straggling, multiple scattering, and detector resolution as a function of depth.

be registered with a final energy *E*. If the energy broadening effects are described as a Gaussian model, the $R_i(x)$ can be expressed as

$$
R_i(x) = \frac{k}{2} \left[erf \left(\frac{E_i + \Delta - \overline{E}(x)}{\sqrt{2}\sigma_{E(x)}} \right) - erf \left(\frac{E_i - \Delta - \overline{E}(x)}{\sqrt{2}\sigma_{E(x)}} \right) \right]
$$

where $\sigma_{E(x)}$ is the standard deviation of the total energy broadening effect for the charged particle with the depth x in the sample. And k is the constant which contains the neutron flux, fractional yield for the charged particle, cross-section for charged particle production, and the detection efficiency. The $R_i(x)$ for 1472 keV alpha particle from the ${}^{10}B(n,\alpha)^7$ Li reaction was integrated for each bin and the contour plot of the integral is shown in Fig. 2. The scale corresponds to the normalized probability. The bin size is 3.5 nm and 1 keV for the depth and energy, respectively. As shown in Fig 1 and 2 the detector energy resolution is dominant within the depth of 0-0.4 μm.

In Fig. 3 predicted NDP spectra are shown for SRM-2137 sample. The depth profile for ^{10}B of the SRM-2137 measured by using the SIMS method is shown in the inset of Fig. 3. The spectrum with energy straggling, multiple small-angle scattering and detector energy resolution was calculated by using the interval average approximation [5]. The Si detector was situated 11 cm from the sample in the normal direction of the sample surface. The active area of the detector was 150 mm^2 , while the neutron beam irradiated area was considered as a point. The circles in Fig. 3 show the TRIM calculation. In the TRIM calculation, the 1472 keV alpha particles were emitted at each depths (0-0.32 μm), and the energies of the transmitted particles were measured. The solid and dashed lines show the predicted spectra. The solid line describes the spectrum where energy straggling and multiple small-angle scattering components of energy broadening were considered, while the spectrum plotted as a dashed line considered the energy broadening of the detector energy resolution additionally. As can be seen in Fig. 3, the energy straggling and multiple small-angle scattering are negligible since all the 10 B is within 0.32 μm of the sample surface. The energy broadening of the SRM-2137 is primarily due to the energy resolution of the detector and associated electronics

4. Conclusion

The contributions to the energy broadening of the NDP spectrum were determined. The standard deviations of the energy broadening effects – energy straggling, multiple small-angle scattering and detector resolution – were calculated as a function of depth. The detector response function for the 1472 keV alpha particle from ${}^{10}B(n,\alpha)^7Li$ reaction in silicon medium was calculated based on a Gaussian model. In addition, the observed NDP energy spectrum was predicted by using the measured 10 B concentration profile.

Fig. 2. Detector response function for the 1472 keV alpha particle in silicon.

Fig. 3. The modeled NDP spectrum for the 1472 keV alpha particle from the SRM-2137 sample. The circles show the TRIM calculation, and the solid line is the spectrum considering $\sigma_{\text{straggling}}$ and $\sigma_{\text{scattering}}$. The dashed line shows the spectrum considering $\sigma_{\text{straggling}}, \sigma_{\text{scattering}}$ and σ_{det} .

The effect of the geometrical acceptance angle for the energy broadening was considered negligible in this study. However, there is a specific area of the neutron beam, so it needs to consider the geometrical effect to derive the detector response function in the real case. In the future, the measured spectrum will be analyzed based on the determined detector response function by using the appropriate deconvolution algorithm.

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