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Simulation of Neutron Induced Charged Particle Spectrum for Neutron Depth Profiling

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1. Introduction

With the revolution of the 4th industry, it is required to guarantee the performance and safety of various ICT (Information and Communication Technology) products such as IoT, autonomous vehicles, and robots. Companies producing ICT products use the advanced measuring equipment to manage their production processes. Therefore, in order to establish a standard for the ICT device production process, top-level technology for quantitative analysis of element should be supported.

In KAERI (Korea Atomic Energy Research Institute), quantitative analysis of doping elements in Si, SiC, and InP substrates and thin films of compounds such as SiGe and IGZO has been conducted using NDP (Neutron Depth Profiling) method. A conventional KAERI-NDP system has been designed and developed at HANARO, a 30 MW research reactor in 2014[1]. The KAERI-NDP system has been developed for various applications of NDP technique. However, the operation of the system has been suspended due to a decrease of the detection limit by neutron flux, a decrease in depth resolution, and a problem in the vacuum system. Currently, the conventional system has been improved to construct a target chamber and detection system dedicated to ICT material analysis.

NDP is based on the illumination of a sample with neutrons. Upon absorption of these neutrons, certain isotopes of light elements undergo exoergic reactions. These reactions create mono-energetic charged particles, and a recoil atom. The depth is obtained from the energy loss of those charged particles escaping surface of substrate material. Energy loss spectrum of charged particle 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. There are various methods to analyze the NDP spectrum. In this study, nuclear reaction between neutron and target nuclide is simulated using Monte Carlo method, and the detection response function is evaluated by calculating the energy loss of charged particles.

2. Methods and Results

In this work, we used MCNP code to simulate details of the NDP process. The MCNP model designed to simulate NDP has a simple geometry with the detector face directly facing the sample. A cold neutron beam with a 1 cm radius is incident on the sample.

The energy spectrum of the cold neutrons transported through the CG1 is determined using the Maxwellian distribution function based on the neutron temperature [2]. Energy differential flux of the neutron beam is shown in figure 1. Average temperature and peak energy of the neutron beam are 26.3 K and 2.3 meV, repectively.

The geometry of the model is described in figure 2. The model includes a silicon charged particle detector with 100 μm thick of sensitive depth and 150 mm^2 of active area, the target, the neutron beam, and a 50 cm diameter aluminum cylindrical chamber. The chamber is filled with a low atmosphere of air.

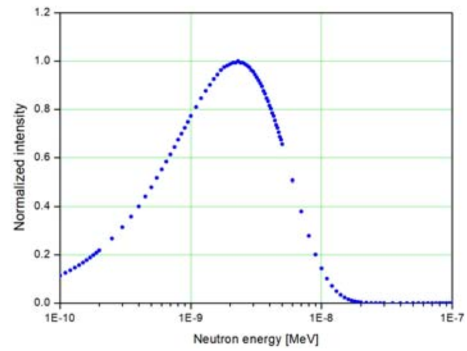

Fig. 1. Energy differential neutron flux of neutron beam

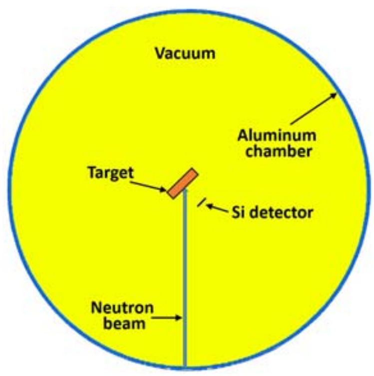

Fig. 2. Geometry of the MCNP model

The target material is Standard Reference Material (SRM) 93a that is often used for an energy calibration of the NDP system. SRM-93a is 6.3 mm thick borosilicate glass with a uniform distribution of B-10 throughout the entire volume. Distance between the SRM-93a sample and the silicon charged detector is 3 cm in the model.

In the MCNP model, neutron, photon, triton, deuteron, He-3, and Alpha particle are considered, and ENDF/B-VII.0 nuclear library is used. In addition, the light and heavy-ion recoil in the particle physics option are employed in the simulations. The NCIA algorithm is used for the proton, deuteron, triton, He-3, and alpha. Detection resolution is considered 14 keV for the FWHM at all energy region using the GEB option of MCNP.

An energy spectrum of neutron induced charged particle and gamma-ray of SRM-93a is shown in figure 3. The figure shows the energy loss spectrum of alpha and Li ion, and it shows the gamma-ray component. When B-10 in SRM-93a absorbs a neutron, it undergoes the following nuclear reaction:

$$^{10}B + n \rightarrow {}^{7}Li^{*} + {}^{4}He(1472.4\,keV)\ (93.7\%)$$
$$^{7}Li^{*} \rightarrow {}^{7}Li(840\,keV) + \gamma(478\,keV)$$
$$^{10}B + n \rightarrow {}^{7}Li(1013\,keV) + {}^{4}He(1776.7\,keV)\ (6.3\%) \quad (1)$$

The figure shows apparent vertical steps in counts at 1776.7 keV, 1472.4 keV, and 840 keV. The step-wise energy spectrum of the SRM-93a can be inferred from the relation between the thickness of the sample and range of the alpha particle. The SRM-93a sample has a uniform B-10 distribution throughout a 6.3 mm thick, and this thickness is longer than the ranges of alpha particles and Li ions emitted from B-10.

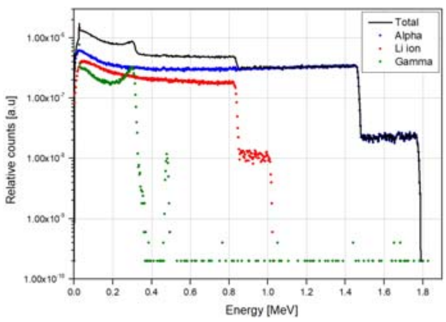

Fig. 3. Simulated neutron induced charged particle spectrum of SRM-93a

A comparison of a spectrum produced by the MCNP model to that of experimental data from the KAERI-NDP system is shown in figure 4. In the figure, it can be seen that the two spectra match well. However, the vertical steps at the energy of 1472.4 keV and 840 keV in measured spectrum are broader than the those in the calculated spectrum. The alpha particle resolution of the measurement is estimated to be 26 keV for the FWHM. The broadening that appears in the experimental data is a result of the energy broadening of the silicon charged detector. The calculated spectrum shows that the MCNP NDP model is accurately modeling the energy broadening of the KARI-NDP system.

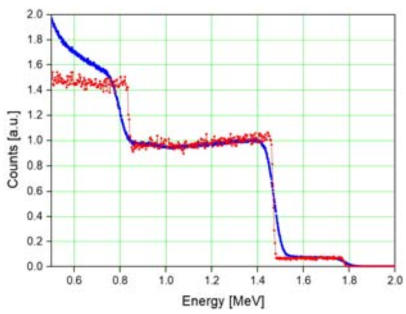

Fig. 4. Comparison of calculated and measured NDP spectra

3. Conclusions

The charged particle energy spectra of the SRM sample was measured and calculated as a test for the performance of the KAERI-NDP system. The simulated NDP spectrum is well agreed with the measured one. The simulation of NDP spectrum is useful for the following: benchmarking ratio of concentrations and shape of distributions for the KAERI-NDP system, validating the spectrum fitting method, optimal design of beam transport system using simulation data, production of training data for NDP spectrum analysis method using artificial intelligence.

Acknowledgement

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