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Evaluation of Monte Carlo Codes Regarding the Calculated Detector Response Function in NDP Method

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1. Introduction

Neutron Depth Profiling (NDP), with another name as Neutron Induced Charged Particle Depth Profiling, is a non-destructive analytical method for determining the concentration (atom.cm^{-3}) of a particular isotope or element as a function of depth from the surface of the sample. The NDP method is useful for measuring the spatial distribution of light elements such as ^{10}B, ^{3}He, ^{6}Li, ^{7}Be, ^{22}Na, etc. in any substrate [1]. The basis of the NDP is the irradiation of a sample with a thermal or cold neutron beam and the subsequent release of charged particles due to neutron-induced exoergic charged particle reactions. Neutrons interact with the nuclei of elements and release mono-energetic charged particles, *e.g.* alpha particles or protons, and recoil atoms. Depth profile of the analyzed element can be obtained by making a linear transformation of the measured energy spectrum by using the stopping power of the sample material. A few micrometer of the material can be analyzed nondestructively, and on the order of 10nm depth resolution can be obtained depending on the material type with NDP method.

In the NDP method, the one first steps of the analytical process is a channel-energy calibration. This calibration is normally made with the experimental measurement of NIST Standard Reference Material sample (SRM-93a). In this study, some Monte Carlo (MC) codes were tried to calculate the Si detector response function when this detector accounted the energy charges particles emitting from an analytical sample. In addition, these MC codes were also tried to calculate the depth distributions of some light elements (^{10}B, ^{3}He, ^{6}Li, etc.) in SRM-93a and SRM-2137 samples. These calculated profiles were compared with the experimental profiles and SIMS profiles [2].

At the present time, it is only a few studies of MC simulation in the NDP method, therefore, the performance of MC codes does not have enough a reliable proof of ability in the NDP simulation. In this study, some popular MC neutron transport codes are tried and tested to calculate the detector response function in the NDP method.

The simulations were modeled based on the real CN-NDP system which is a part of Cold Neutron Activation Station (CONAS) at HANARO (KAERI) [3].

2. Monte Carlo neutron transport codes and technique

Several Monte Carlo all-particle transport codes are under active development around the world. Each of these codes inherits and exchanges the properties, capacities, and nuclear data from other codes and may have lacked some important features [4]. Because the focus response function was focus of this study so some popular MC neutron transport codes, such as MCNP6 [5], GEANT4 [6], PHITS [7], and FLUKA [8], were adopted of this testing.

3. NDP System

The CN-NDP system has been installed at the end of the CG1 neutron guide of HANARO. The CN-NDP system consist of a sample chamber, charged particle detectors, neutron beam collimator, beam stopper, quick shutter, and NIM electronic modules for accounting the charged particle. The cross section of CN-NDP system is shown in Fig. 1. The body chamber was constructed from SUS304 type stainless steel. The body is a cylinder with a 60 cm diameter, 31.5 cm height, and 1 cm thickness. The base plate of the UHV chamber is made of the same type stainless steel with a 68 cm diameter and 2 m thickness. On the top of the UHV chamber, the 6061 aluminum alloy lid plate with a 68 cm diameter and 2.5 cm thickness is used to close this chamber when changing the analytical sample or correcting the silicon surface barrier detectors. The UHV chamber consists of five large identical flanges and six small identical flanges with each pair of flanges creating perpendicular pathways through the UHV chamber. The large flanges have a 9.75 cm inner diameter and 10.16 outer diameters. The neutron beams in/out windows were sealed off with 0.13 mm thickness aluminum so that the chamber may be evacuated without causing noticeable neutron interference and two monitor flanges sealed by thick glass. Three small flanges with a 3.4 cm inner diameter and 3.81 cm outer diameter are connected with gauges, gas purring, convection gauge, electronic feed-through, etc. The other three small flanges that are not in use for the CN-NDP system were sealed off with thick aluminum caps. The caps are removable if necessary.

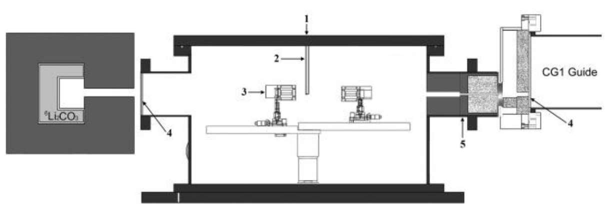


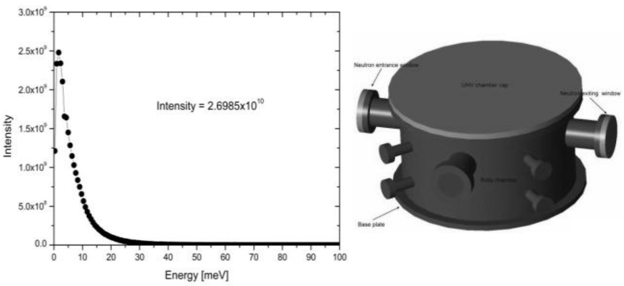
Fig 1. The schematic diagram of a cross-section of CN-NDP system. (1) sample chamber, (2) sample holder, (3) detector holder, (4) Aluminum window, (5) collimator.

An ORTEC ion-implanted Si detector (Model BU-014-150-100) with an active area as 150 mm^2 is used to measure the alpha spectrum from the SRM-93a and SRM-2137 samples when these samples are irradiated by cold neutron beam. The counting time in this experiment was set as 50k seconds. The pulse-height energy spectrum of charged particles is accounted by using MAESTRO-32 software.

4. Experiment and simulations

4.1 Cold neutron flux

The energy and wavelength spectra of the cold neutron beam at the end of CG1 guide were calculated by using McStas code [9] and was shown in Fig. 2a. The total neutron flux at the end of CG1 guide as $9x10^8$ $n.cm^{-2}s^{-1}$ was calculated by integrating the differential neutron flux distribution in the range of 0 to 30Å while the measured neutron flux was about $2.55x10^8$ $n.cm^{-2}s^{-1}$ by activation the gold foil. The discrepancy between experiment and calculation due to the missing of some real factors and conditions of the neutron guide in the McStas simulation.



. (a) (b)

Fig 1. (a) The 2-dimensional neutron distribution as the cold neutron source in NDP simulations. (b) The UHV sample chamber model by using MCAM tool.

4.2 Modeling and simulations

The UHV sample chamber was modeled by MC codes with some simplifies of the specifications that were described in the previous section. Some useful geometry tools as MCAM, CAD2MCsc, and SimpleGEO were applied to render the geometry of CN-NDP system corresponding with each MC code. The UHV sample chamber model showing in Fig. 2b was rendered by using MCAM tool, and this model will be used to NDP simulation.

In the simulation model, a 100 μm thick silicon photodiode detector was modeled as a cylinder shape, which was made of silicon material, with diameters of 13.8 mm. The UHV sample chamber was filled with extremely low atmosphere of air about $2x10^{-4}$ Pa pressure and room temperature to provide vacuum environment. The dimensions of NIST samples were modeled as a 2 μm thick borosilicate wafer with a diameter of 3 cm. The boron material is homogeneously distributed inside the SRM 93a sample model with an implantation dose of 6.2 $\mu g/cm^2$. This SRM 93a sample was chosen because it is often used for the alpha energy calibration of the NDP. Profiling of this SRM 93a sample measures the energy spectra of two alpha particles emitted after neutron absorption. An alpha particle with 1471.76 keV is emitted 93.7% of the time while an alpha with 1775.87 keV is emitted the other 6.3%. The objective of modeling this sample was to compare the measured alpha spectrum generated by assessing SRM 93a sample from the experiment in the Fig. 3.

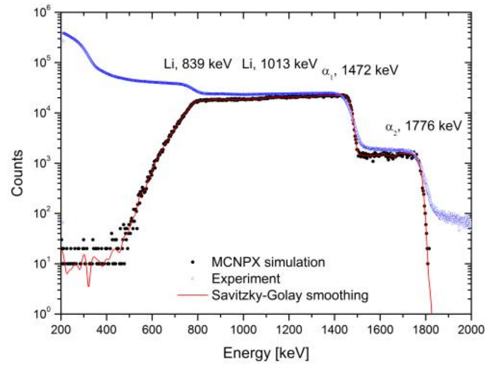


Fig 4. The simulated alpha spectrum and experiment of SRM 93a.

The relationship between the thickness of the SRM-93a sample and the ranges of the charged particles explained the energy spectra in the step-wise shapes. The simulated spectrum almost matched with the measured spectrum except in the low energy region from 0 to 750 keV. The extraneous peak in this energy region of the measured spectrum was considered to be a background noise as gamma rays and energetic electron.

4. Conclusions

The MC simulations are very successful at predicting the alpha peaks in the measured energy spectrum. The net area difference between the measured and predicted alpha peaks are less than 1%. A possible explanation might be bad cross section data set usage in the MC codes for the transport of low energetic lithium atoms inside the silicon substrate. On the other hand, backscattering gamma particles were predicted very well in the low energy region of the spectrum. Based on these results, it can be concluded that MC codes can be used as a simulation toolkit for neutron depth profiling analysis of samples containing ^{10}B element to verify the experimental results.

Acknowledgment

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