GAMMA RAYS FROM MAJOR ELEMENTS BY THERMAL NEUTRON CAPTURE REACTIONS: EXPERIMENT AND SIMULATION FOR PLANETARY GAMMA-RAY SPECTROSCOPY.

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Introduction: The elemental composition of planetary surface can be determined by remotely measuring the energies and intensities of gamma rays that leak out of the surface. Gamma rays are emitted from the surface nuclei which are excited either naturally or by the exposure to cosmic rays and the subsequent interaction of the secondary neutrons [1].

In order to calibrate the gamma-ray intensities to elemental abundance on the surface, one needs to know the production rate of line gamma rays, which is a function of the abundance of element of gamma-ray origin as well as neutron fluxes. The continuum in the energy spectrum is also important to simulate for the estimation of the noise level, counting rate, and detection threshold. Only computer simulation can provide such information and the precision of an observation rely on it. Therefore, it is essential to verify the computer simulation with ground experiments for high-precision missions such as SELENE [2], MESSENGER and BepiColombo [3]. In this work, production and detection of gamma rays from major elements by thermal neutron captures are simulated experimentally and numerically, and the results are discussed.

Experiments: Thermal neutron beams were irradiated to samples at Japan Research Reactor No.3 (JRR-3) at Japan Atomic Energy Research Institute (JAERI) [4]. With nominal flux of ~10^7 /cm^2 sec and beam cross section of 20 x 20 mm^2, thermal neutrons are irradiated to various targets including single-element targets as well as multiple-element targets like a stone. Gamma rays, emitted from a high-purity Fe target which measures 10 x 10 mm^2 and an Al target which measures 13.5 x 13.75 mm^2, are observed with a HPGe detector with a volume of ~110 cm^3. The Ge detector is surrounded with BGO detectors to constitute an anticoincidence system. The thermal neutron capture cross sections are ~barns for Fe, and ~barns for Al, respectively. The atmosphere is filled with He gas to avoid neutron reactions with N in air.

Calculations: The computer simulations need to reproduce variety of interaction and complex geometry of a detector system in a unified manner. For this reason a Monte Carlo computer simulation code Geant4 release 6.2 was chosen to calculate production, transport, and reaction of neutrons and gamma rays [5]. The first calculation is conducted thoroughly from thermal neutron transport to energy deposition of gamma rays in the Ge crystal using the hadronic physics list “QGSP_HP”. Fig. 1 shows a calculated energy spectrum of gamma rays emitted from the Fe target, together with the one by the Ge detector in the experiment. The spectrum by the calculation has few discrete gamma-ray peaks, and it has a continuum while the Fe target is ~0.11 cm thick. The same tendency has been found in other targets and in calculations by MCNPX. Note that in Fig.1, the emission spectrum from the target is shown as a calculation result in order to emphasize a serious difference from the experiment, even though the Geant4 code can provide a spectrum based on energy deposit of gamma rays in a Ge crystal. It is clear that there is a discrepancy in calculating gamma-ray production rates.

Evasion of the problem: Counting rate of a certain gamma-ray peak observed by a spectrometer can be expressed as

\[ C = \frac{M}{A} \cdot N_A \cdot \phi \cdot \sigma \cdot \eta(E_p) \cdot \epsilon(E_p) \]

where M is the mass of the target material exposed to neutron flux, A is the atomic number of the element of interest, N_A is the Avogadro number, b is the isotope ratio, \( \phi \) is the thermal neutron flux, \( \sigma \) is the cross section of thermal neutron capture reaction, \( \eta(E_p) \) is the branching ratio to a channel of \( E_p \), and \( \epsilon \) is the absolute peak detection efficiency. In the computer simulation, capture reaction rates can be calculated properly. By applying the branching ratios to the capture reaction rate outside of the simulation code, it is possible to retrieve the correct gamma-ray production rates. Then the calculation can be restarted by producing gamma rays and let them trans-
port and react, with initial energies determined by the outside multiplication and initial locations where neutron capture reaction took place. The initial directions of produced gamma rays are assumed to be isotropic.

Results and Discussions: Calculated peak gamma-ray intensities observed by the Ge detector are compared with experimental results after employing the evasion method described above. The ratios of experimental results to calculations are shown in Fig. 2, where the major peaks from Fe and Al targets are represented. The ratios are normalized at 352 keV for Fe and 1779 keV for Al because of a neutron flux ambiguity. The error bars are attributed to the experiments. As can be seen from the figure, peak gamma-ray intensities observed in the beam experiments are well reproduced by the calculation method. The ratios of the experimental results to the calculation are 100.0% at 1260 keV, 99.7% at 1613 keV, and 98.3% at 4218 keV for the Fe target, and 100.0% at 4734 keV, 99.4% at 2590 keV, and 99.1% at 983 keV for the Al target. Most of other strong peaks are consistent within the error of ~8%, except for the higher energy doublets from Fe at 7631 and 7646 keV, where more extensive analyses of experimental data are required due to the interference with each other. Even though this method is an indirect way and does not satisfy the requirement of simulating gamma-ray spectroscopy in a unified manner, the method is confirmed to be reliable to reproduce gamma-ray peaks from thermal neutron capture reactions. Comparison of other major elements should be made by using other targets, including stone targets, whose elemental abundances are more resemble with those on the planetary surfaces.