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Simulation study on various physical models of inorganic material

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1. Introduction

High-Z metal elements have been used for radiation shielding as a basic method, most of which are rare earth elements, including X-ray shielding [1]. However, there are two problems; supplying depends on a few specific countries [2], and environmental pollution occurs during the process of mining and separating rare earths [3]. Lead, which is widely used as a shielding material as a non-rare metal, also has problems with environmental pollution and accumulation of heavy metals in the body [4]. To solve this problem, research on shielding materials using organic polymer materials is ongoing [5].

The key to radiation shielding is to increase the radiation absorption rate, and films with a combination of metal and organic materials with a copolymer structure are being used as alternative materials to achieve this purpose [6]. In addition, multi-films in the form of very thin metal films of other metals (such as Co) deposited on a metal oxide substrate (MgO, etc.) are being studied as materials for X-ray energy absorption and optical emission [7]. When X-rays enter the film, some of the energy is absorbed and the rest is reflected or transmitted. In this case, the linear attenuation coefficient is derived by reverse calculating the ratio of the absorbed energy to the transmitted energy [8]. This value shows characteristic values depending on the type and density of the material.

Therefore, in this study, a code was developed to simulate the X-ray generator and film target by representing the geometry, physical model, and radiation source using Geant4 to improve the reproducibility of the X-ray generator used in previous simulation studies by complementing each of their shortcomings. In addition, the simulation results obtained by applying different physical models were compared with the actual measurement values in terms of both the wavelength of the X-rays generated and the amount of energy (absorption, transmission) that reacts with the material, and the most suitable model was selected. A comparative verification study was also conducted on the actual organic-inorganic composite film produced.

2. Materials and Results

2.1 X-ray Tube Model Design

To perform this study, a simulation was designed using the Geant4 toolkit (version 11.1.0) to simulate the X-ray tube. In the case of physical models, models that can closely simulate X-ray bremsstrahlung were selected (Table 1). The intensity of the electron beam entering the anode was simulated in a way that mimics 150kV X-ray equipment. Tungsten was used as the material for the anode that generates X-rays when hit by the electron beam, and its thickness was set to 2mm. The tungsten anode was designed to have a parallelogram structure with a slope of 12 degrees based on the geometry reproduced in previous studies, which is the same shape.

The design of the geometry that simulates the overall X-ray tube is shown in Fig. 1. In addition to the parts described earlier, the lead collimator and Al filters attached to the emission part of the X-ray tube were also simulated by referring to the geometry designed in G4XRTube.

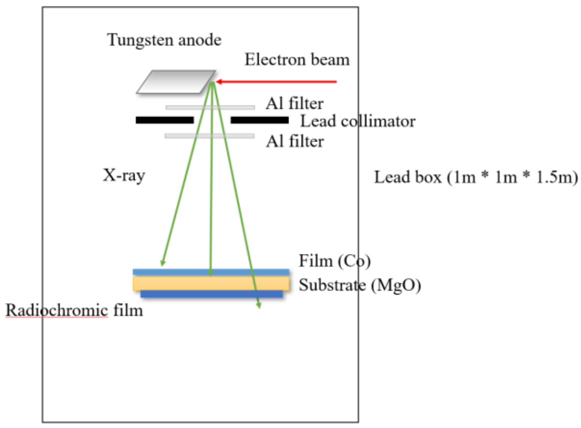

Fig. 1. Output current of the SiC detector for three particles that have been simulated as interacting in the detector randomly in time, with an average event rate of 108 events/s.

2.2 Inorganic Film Design

The Irradiated material that measures the energy absorption and transmission of inorganic materials in the simulation performed a comparative analysis by referring to the geometry and data presented in Piamonteze's 2020 paper [7]. First, the geometry of the entire film was taken as a combination of a 2nm-thick Co film deposited on a 0.5mm-thick MgO substrate.

The simulation estimated the amount of X-rays incident on the film, the amount of absorption, reflection, and transmission in relation to the incident amount, using various physical models applied to the geometry of the mixed film, and utilizing bremsstrahlung radiation and characteristic radiation generated at 150kV.

2.3 Result of X-ray Generating Accuracy

We first conducted a comparison between the wavelength ranges of characteristic and bremsstrahlung x-rays generated from different models and the measured values. The reported characteristic x-ray wavelengths for tungsten were 57.98 and 59.32 keV, and for the bremsstrahlung x-ray range, we referred to data from previous actual investigation. As a result, a distribution difference about characteristic radiation value between the experimental and simulation values was observed in Fig. 2.

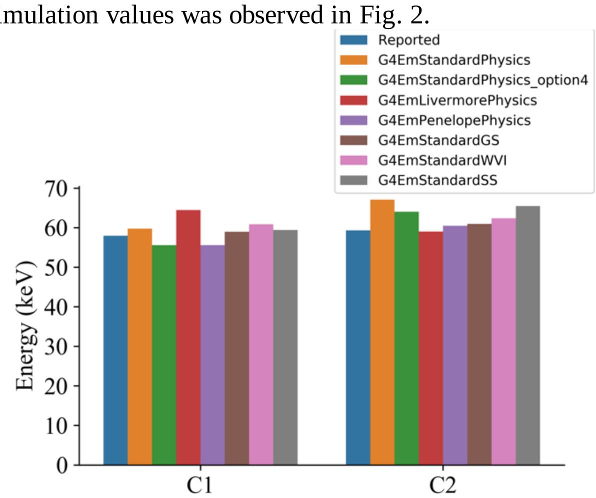

Fig. 2. The X-ray output spectra from characteristic radiation, compared with the empirical data (reported) and the simulation data (other models starts with 'G4'). C1: lower characteristic radiation energy, C2: higher characteristic radiation energy.

2.4 Result of X-ray Absorbance Accuracy

Comparison data regarding the amount of energy absorbed, and transmitted when the material is irradiated by X-rays were also compared with data from previous empirical papers. In those previous empirical or simulation papers, lead-scintillator was used as the material to measure the extent of energy absorption and transmission. Thus, in this paper as well, simulations were conducted using the same material adopted from those studies.

For the inorganic material Co-MgO film, it was confirmed that the G4EmStandardGS model best describes the absorption, transmission, and reflection of X-rays (Fig. 3). In the comparison between the basic models, option4 better explained the measured values than the basic G4EMStandard.

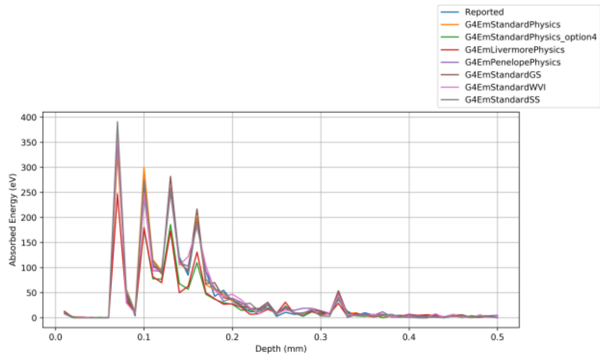

Fig 3. The absorbance data of Co film-MgO substrate material, for seven physics models. The x axis stands for every 0.1mm in the substrate.

3. Conclusions

In this research, we presented the geometry of an appropriate X-ray tube model through Fig. 1, and showed through Fig. 2 and Fig. 3 that the model relatively well simulates X-ray radiation physics phenomena by comparing it with actual measurement data. In the future, this research can be used as basic data for calculating the energy absorption rate of X-rays for inorganic films. Also, as the additional effects, the simulation geometry design approach derived from this study can also help design X-ray tubes more efficiently to deliver X-rays that are reflected more effectively to the target material. Moreover, by obtaining almost the same results with fewer simulations according to the findings presented in this study, it is possible to reduce the time and computational effort required if further researches will be supported.

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