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Modeling and Simulation of the Electron Beam Cured Polyester using Geant4

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Abstract - The electron beam curing process is a technology that can shorten the curing time and improve the mechanical strength of materials. Modeling and simulation of electron beam irradiation process can identify product problems in advance and shorten development time. In this study, the electron beam curing process was modeled and simulated using Geant4 and compared with the actual specimens cured with electron beam irradiation. Among the forms of energy deposition to the sample, it was confirmed that the electron ionization is a major factor in curing. It was found that the surrounding environment, such as the substrate supporting the specimen, should also be a factor that cannot be ignored in the electron beam irradiation process. The results of this study can be used as basic data for all processes using radiation.

Key words : Electron beam, Curing, Modeling and simulation, Geant4

INTRODUCTION

Electron beam curing technique is used in various industrial fields such as coating (Kumar and Sasaki 2013), adhesives (Ebe *et al*. 2003) fabrication of plastic (Nishitsuji *et al*. 2007) and composite (Zhang *et al*. 2002) materials. This technique versus conventional curing system provides a fast curing process (Chakabort *et al*. 2011) with low energy consumption, and the high physical performance. The electron beam accelerator is a radiation generator that can deliver a lot of energy in a short time, and industrially allowed up to 10 MeV (Berejka and Eberle 2002). In order to guarantee a uniform degree of curing, it is necessary to accurately analyze the deposited energy distribution by electron beam (Xiong *et al*. 2018). The increase in product shape complexity makes it difficult to represent the irradiation dose distribution by simple calculations (Zhao *et al*. 2015). As it is difficult to predict what kind of consequences will occur on the quality of the product due to local non-uniformity, the development of countermeasures is required.

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Geant4 is a program that can model and simulate the reaction with materials for various radiation sources such as alpha, beta, gamma and neutrons (Kang and Kim 2007). Although it is an open library based on C++, it has been verified over a long period of time and is continuously developing, and it provides various physical models (Agostinelli 2003). In this study, a curing process that can be performed with radiation, especially electron beams, was modeled and simulated using Geant4, and compared with actual cured matrix resins with electron beam. The physical type of radiation deposited energy and the surrounding environment was considered as key factors to analyze the curing process. It could be extended to basic data for manufacturing composite materials using electron beam.

EXPERIMENTAL METHODS

1. Modeling and Simulation

A cylindrical electron beam curable resin with a diameter of 10 cm and a height of 10 cm was modeled using GEANT4 code. The resin material was set to a density of 1.1 $g \cdot cm^{-3}$

with the element ratio of hydrogen 4, carbon 10 and oxygen 4 based on polyester. A plate-shaped Fe substrate was placed directly under the resin sample. The physical model applied to the simulation is QBBC_PEN, which is known as an appropriate model for 10 MeV electron beams (Miloichikova *et al*. 2019). The default Cut value of GEANT4 is 1 mm, but 1 μm was used to simulate to obtain the realistic data. A point and a plane (20 × 20 cm) electron beam were implemented on 5 cm in the vertical direction of a cylindrical sample using a GPS (General Particle Source) macro file. The energy of the electron beam was 10 MeV, and the number of beam on was 10,000,000. The total deposited energy was scored into 100 × 100 matrix by dividing the primary energy at the reacting step generation. Each step process name such as eIoni, eBrem, compt, phot and msc that is corresponding to the electron ionization, electron Bremsstrahlung, Compton scattering and photoelectric generates independent scoring files.

2. Electron beam curing of polyester resin

Carboxylate polyester acrylate (PN-5600, Polynetron, Korea) was used as an electron beam curable resin. This resin has the advantage that it is easy to predict the irradiation dose as the color changes to brown visually every time it is scanned using an electron beam accelerator. The color change of the resin according to the number of scans is shown in Fig. 1, and the thickness of each specimen is approximately 1 cm. A specimen of the same size as the simulation was produced using a very thin polyethylene barrel. It was scanned 5 times using a 10 MeV electron beam accelerator, and the photograph of the manufactured specimen can be seen in Fig. 6. Beam current was 3 mA, and scanning speed was 1.06 $m \cdot min^{-1}$.

RESULTS AND DISCUSSION

1. Simulation result with point source

The QBBC_PEN physical model can generate a wide variety of processes. The 10 MeV electron beam directly generates electron ionization and electron Bremsstrahlung, multiple scattering through the polyester specimen in this physical model. By generating gamma rays as secondary effects, Compton scattering and photoelectric effects generated. In the simulation results, Fig. 2 shows the probability distribution of deposited energy (xz plane) by one electron, and it is possible to compare the relative amounts for each process rather than the absolute value.

The energy at the source was 10 MeV and the total deposited energy was 9.64 MeV, indicating the presence of scattering in the air from the source to the sample and the energy that escaped without deposition among the energy incident on the sample. The direct electron ionization (9.48 MeV) process plays a dominant role in the total deposited energy. MSC (Multiple scattering) process exists for continuity rather than physical importance as the way programs process data during simulation. Reducing the cut value can also reduce the total amount processed by MSC. The effect of other processes can be also observed, but this is very small compared to the direct ionization by electrons, so the effect on the curing will be negligible.

2. Simulation result with plane source

Fig. 3 shows the distribution of deposited energy when the sample is viewed from above. This is the sum of the z-axis values for the xy plane matrix, and is the same condition as when the actual specimen is viewed from above.

The total deposited energy of 0.78 MeV is because the area of the plane source is larger than that of the sample. By setting the size of the plane source to be wide, the energy reflected from the substrate at the bottom of the sample was considered. A uniform deposited energy is observed around 6 cm in diameter from the center of the circle, but the energy gradually decreases on the outside ($0 < x < 2, 8 < x < 10$), and at the boundary ($x = 0, 10$), the value is about half compared to the center.

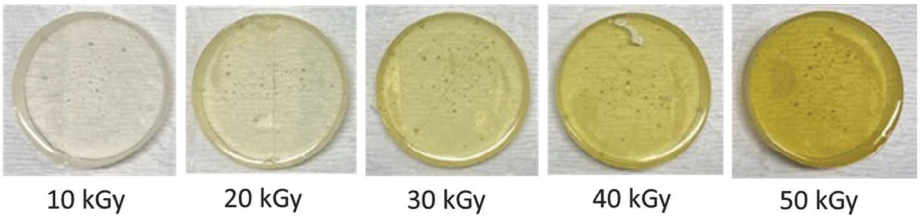

Fig. 1. Color change per scan of the electron beam for polyester acrylate resin. 10 kGy irradiated per scan on the samples.

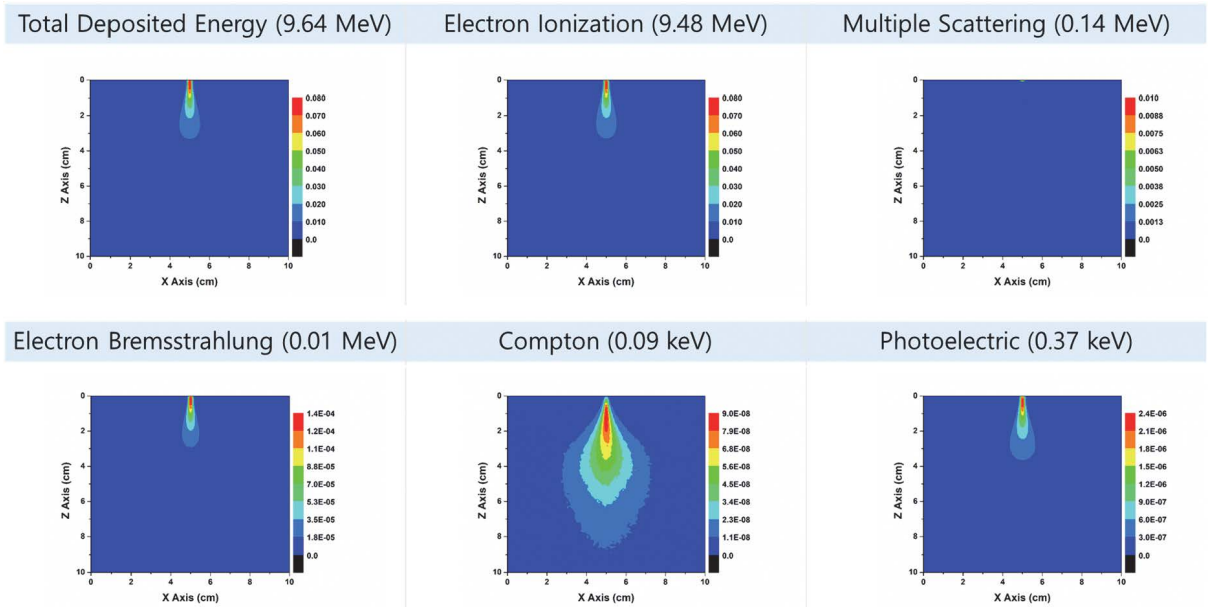

Fig. 2. Simulated deposited energy distribution by point source. The energy value next to each process name represents the sum of the data values.

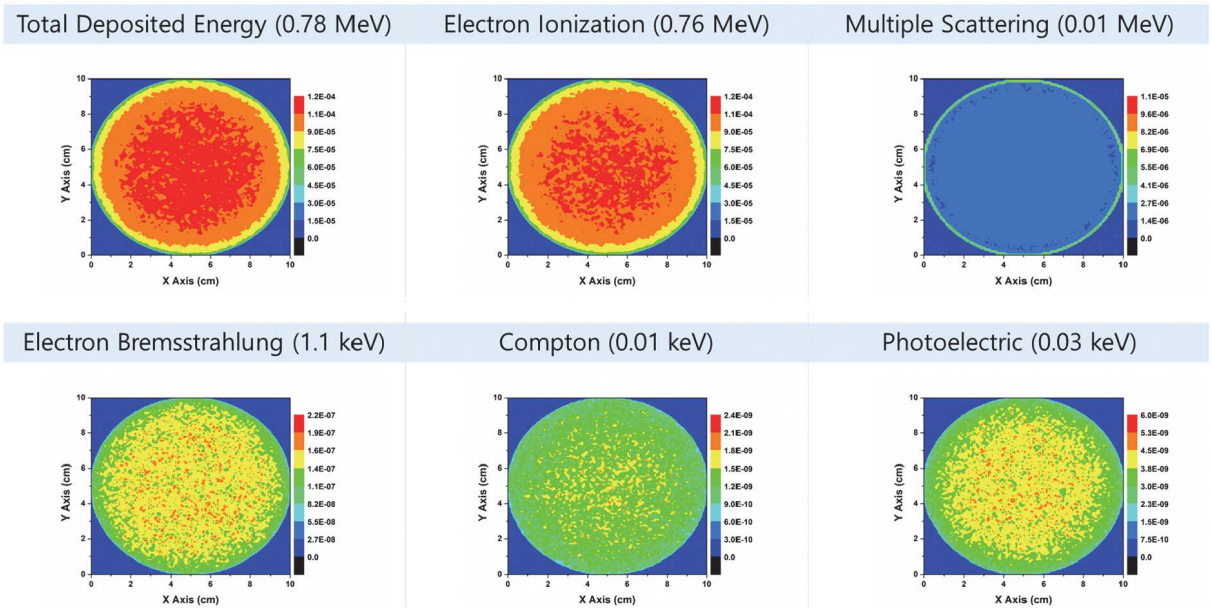

Fig. 3. Simulated deposited energy distribution by plane source on xy plane. The energy value next to each process name represents the sum of the data values.

For each process, the direct electron ionization is the dominant factor for deposited energy, similar to the results in the point source. At the boundary of the sample, the simulation program processed the progress of radiation in MSC. Compared with other processes, it can be seen that Compton scattering occurs evenly inside. Although locally high values are observed in electron Bremsstrahlung and photoelectric, they are also negligible compared to electron ionization.

Fig. 4 shows the deposited energy distribution for the vertical cross section (xz plane) of the sample. At the midpoint of the sample ($3<x<7$, $2<z<3$), a place where the energy was concentrated appeared. These characteristics are very different from the point source simulation results. There are some differences, but similar characteristics appear for each

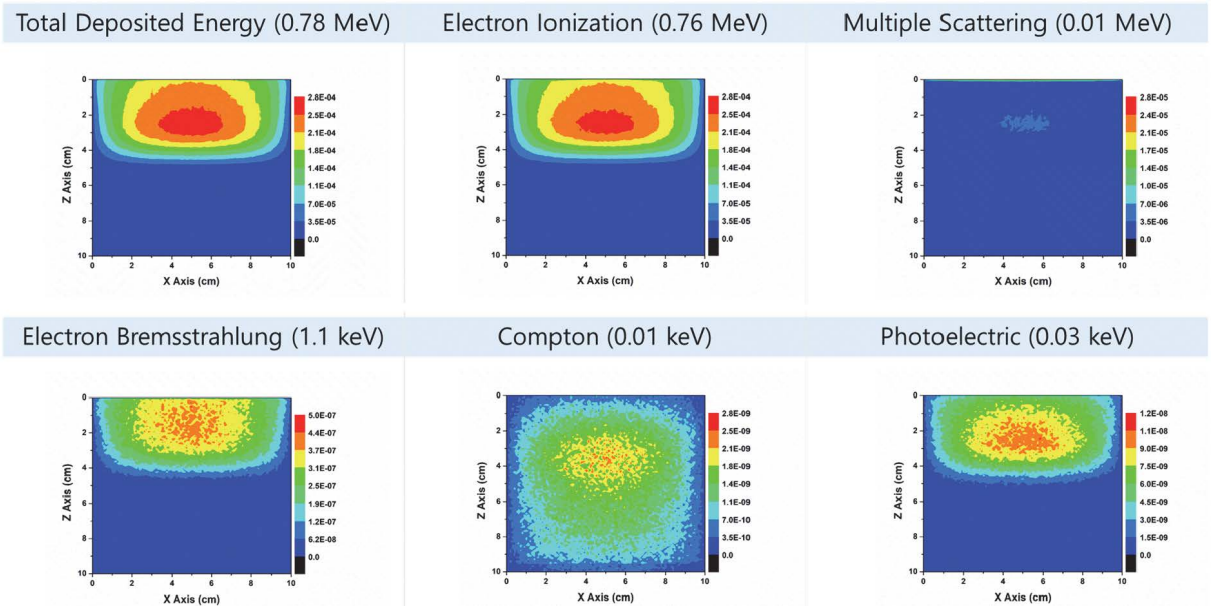

Fig. 4. Simulated deposited energy distribution by plane source on xz plane. The energy value next to each process name represents the sum of the data values.

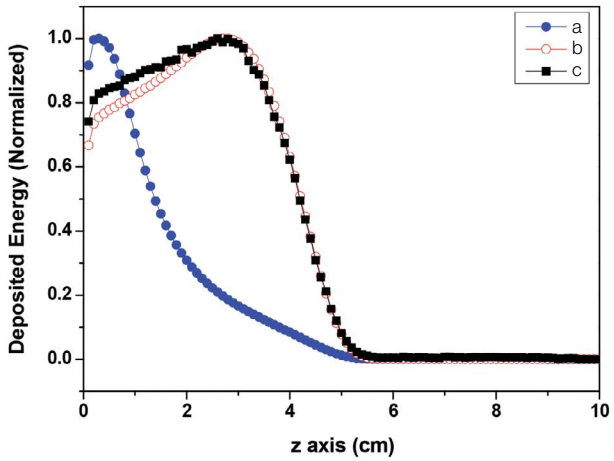

Fig. 5. Simulated deposition energy distribution on the polyester resin by 10 MeV electron beam. (a) is by point source, (b) is deposited energy sum in xy plane from point source, and (c) is by plane source.

process.

The energy profile extracted from the middle of the vertical direction (x = 5) with respect to the z-axis was normalized and compared in Fig. 5. In both point and plane sources, little energy is deposited above 5 cm. However, the place where the peak of the deposited energy appears is 0.5 cm in the point source and around 3 cm in the plane source. It should be considered that the scattering increases in the xy plane as the penetration depth of the electron beam of the point source increases. Therefore, the sum of the energy on xy plane with respect to the z axis direction of point source was obtained as shown in Fig. 5(b). This result became similar to that of the plane source in Fig. 5(c).

3. Electron beam cured resin

Fig. 6 shows a photograph of the specimen cured using electron beams in the same size as in the simulation. As shown in Fig. 1, the color distribution of the specimen is assumed to be proportional to the deposited energy based on the change according to the irradiation dose. The photograph of top view is similar to the simulation result in Fig. 3, and side view is the same as result in Fig. 4. Therefore, we can infer that a linear relationship is maintained between the deposited energy and the degree of browning of the specimen, and we believe that the simulation results can represent the actual curing of the specimen.

In the actual specimen (Fig. 6(b)), curing occurred at the boundary about 1 cm in the region of $6 < z < 10$ cm where almost no energy was deposited in the Fig. 4 simulation. In other words, the inside of lower 5 cm of Fig. 6(b) was remained in liquid form without curing. We extracted the cumulative data for this region from the simulation result in Fig. 4 and represent in Fig. 7. This result shows that the energy deposited on the boundary of the specimen is relatively larger compared to the center. This energy distribution

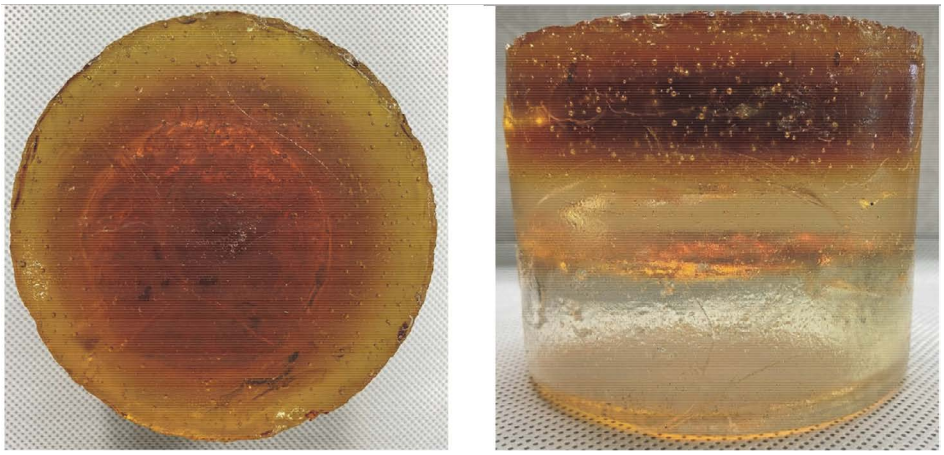

Fig. 6. A photograph of electron beam cured polyester resin that has same dimension with simulation. (a) is top view and (b) is side view.

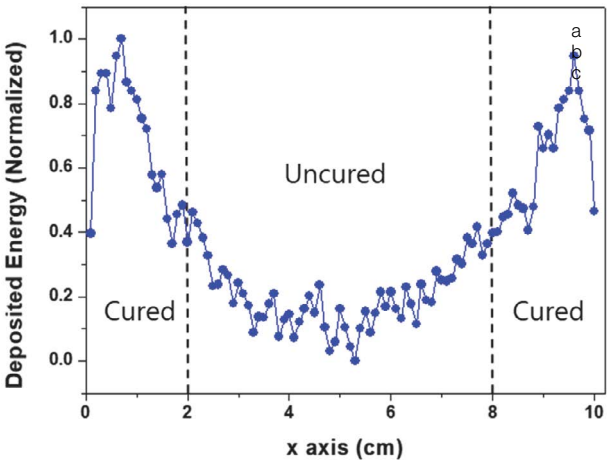

Fig. 7. Sum of extracted data in range of $6 < z < 10$ of total deposited energy in Fig. 4.

does not occur when the underlying substrate is not present. Therefore, we think that the lower 5 cm is the radiation reflected from the substrate and incident to the side of specimen. It can be seen that the surrounding environment in which the specimen is placed affected radiation curing.

CONCLUSION

In this paper, the deposited energy distribution was and simulated using Geant4 when 10 MeV electron beams irradiated on a polyester resin. The deposited energy depth of the electron beam was about 5 cm, which was mainly due to the electron ionization process in simulation results. In addition, the actual electron beam curing and simulation were very similar. These results confirmed that Geant4 simulation is possible to modify the electron beam curing process.

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