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Extended Algorithm for Simulation of Light Transport in Single Crystal Scintillation Detectors for S(T)EM

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Summary: The new extended Monte Carlo (MC) simulation method for photon transport in S(T)EM back scattered electron (BSE) scintillation detection systems of various shapes is presented in this paper. The method makes use of the random generation of photon emission from a scintillator luminescent centre and describes the trajectory of photons and the efficiency of their transport toward the photocathode of the photomultiplier tube. The paper explains a new algorithm for determining the position of interaction of the photon with the surface of the single crystal scintillator or of the light guide with nearly arbitrary shapes. Some examples of the utilization of the simulation method are also included, and conclusions for very simple edge-guided signal (EGS) scintillation detection systems made. The computer optimized design of the BSE scintillation detector for the S 4000 Hitachi SEM was chosen to demonstrate the capability of this MC simulation method. SCANNING 29: 249–253, 2007. © 2007 Wiley Periodicals, Inc.

Key words: Monte Carlo simulation, photon transport, scintillation detector, single crystal scintillator, light-guide, signal processing, SEM, S(T)EM

Introduction

In S(T)EM, the Everhart-Thornley (ET) scintillation detection system (Everhart and Thornley 1960) is often used for detection in the back scattered electron (BSE) image mode. A lot of papers are engaged in the study of scintillators (Pawley, 1974, Autrata *et al*., 1978, 1983a, 1983b; Robbins, 1980) and of photon collection (Baranov *et al*., 1996; Huber *et al*., 1999; D'Ambrosio *et al*., 1999), but little attention has been paid to the photon transport efficiency in relatively complex BSE scintillation detection systems. The inefficient transport of photons emitted from luminescent centers through a scintillation detector of electrons is a frequent cause of poor S(T)EM images, particularly in the BSE image mode. In such cases, edge-guided signal (EGS) scintillation systems that utilize a signal from the side of a scintillator, and have a complicated geometry, are often used. The best way to avoid the light-guiding problems of these systems is Monte Carlo (MC) simulation of signal photon transport. Unfortunately, the previous code SCINTIL (Schauer and Autrata, 1992) developed in our laboratory was built using an algorithm for rotationally symmetric systems where a function of one variable coordinate was used. Therefore, the extended code SCIUNI, intended for practically any geometry, has been developed and its features are presented in this paper.

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Extended Model of Monte Carlo Simulation

The new extended simulation method is based on the SCINTIL code (Schauer and Autrata, 1992) for the rotationally symmetric systems. The MC method repeatedly (10^4–10^6 times) makes use of random generation of photon emission from a luminescent centre and describes the trajectory and the efficiency of the photon transport to the photocathode of the photomultiplier tube (PMT). For each segment of the trajectory the following physical processes (included in the simulation program) are calculated: (i) determination of the position of interaction of the photon with the surface of the scintillator or of the light guide, (ii) calculation of the photon absorption in the volume of a particular material, and (iii) determination of the mirror reflection from a metal coated surface or of the Fresnel reflection from or passage through a polished surface or of the diffusion reflection from or passage through a matted surface.

Each segment of the photon trajectory is given by two subsequent interactions of the photon with the scintillator or light-guide surfaces. The significant extension of the new model consists in a new extended description of detector surfaces and subsequently in the determination of the position of photon interaction with the surface of the scintillator or of the light guide. In the extended model, any surface can be described by a very simple equation:

$$\sum_{i=1}^{3} k_i \frac{(x_i - x_{0i})^2}{A_i^2} = P \qquad (1)$$

where x_1, x_2 and x_3 are the x, y and z intersection point coordinates, x_{01}, x_{02} and x_{03} are the x, y and z surface body origin coordinates, and $k_1, k_2, k_3, A_1, A_2, A_3$ and P are geometrical coefficients of the surface as described for different bodies in Table I.

Using the individual trajectory segments, it is possible to determine the photon transport efficiency at a position of primary electron impact on the scintillator surface. Besides this, further quantitative information such as light intensity distribution or direction of photon propagation at the light-guide output can be obtained using this simulation method. Algorithms for this extended MC simulation method have been incorporated in the 3.0 version of SCIUNI program, which also involves new loops for the light-guide shape optimization. So, the computer optimized design (COD) of nearly any scintillation detection system for S(T)EM can be performed using this version of SCIUNI. The source code of the program SCIUNI has been written in Fortran 77 and compiled on different computer platforms. At present, versions for UNIX and Windows operating systems are available. The simulation results presented in this paper have been obtained using BSDi UNIX operating system.

TABLE I. Some examples of coefficients for different lateral areas for Equation (1)

Body/coefficient	A_1	A_2	A_3	k_1	k_2	k_3	P
Sphere (any axis)	r	r	r	1	1	1	1
Cone (y axis)	r	v	r	1	−1	1	0
Cylinder (x axis)	1	r	r	0	1	1	1
Plane ($\perp z$ axis)	1	1	1	0	0	1	0
Plane (deflection from z axis)	k	1	1	1	0	−1	0
Ellipsoid (y axis)	a	c	a	1	1	1	1
Hyperboloid (x axis)	c	a	a	−1	1	1	1

r = radius, v = body high, k = slope of deflection, a = half-axis (plane of symmetry), c = half-axis (along body axis).

Typical Results for SCIUNI Simulations

Some image modes of S(T)EM require that the electron impact active surface of the detector of signal electrons should be fitted into a very small space, mostly symmetrically around the primary electron beam. This demand is easily fulfilled for semiconductor or channel plate detectors. However, they possess low detective quantum efficiency and/or a high decay time, so that they are often unusable. Therefore, scintillation detectors in nonclassical arrangements are applied. Here, the signal must be guided through an edge of a plate scintillator (Bauer and Egg, 1984). The input end of the light guide must be narrow to match to the edge of the scintillator; and the output end may be enlarged, according to the input window of the photomultiplier. The design of such a scintillator–light-guide system with a high efficiency of the light transport is the key problem of the detector design. Generally, the efficiency of these EGS scintillation detectors is very hard to estimate. Owing to the low symmetry of EGS detection systems, the efficiency can hardly be calculated analytically. For this reason, the MC simulation method is a very useful tool.

Examples of the MC simulation method, i.e. the results of modeling very simple EGS scintillation detector configurations, are shown in Figure 1. The YAG:Ce single crystal and polymethyl-methacrylate (PMMA) were materials used for scintillators and light guides, respectively. Two shapes of scintillators with Al deposited electron impact surfaces, in combination with three shapes of light guides, were tested. The output edge of the scintillator was connected to the input end of the light guide by using optical cement. The circular and the square profiles of scintillators were 20 mm in diameter and side length, respectively. All light guides were 60 mm long. The design of the simulated detection system is viewed at each graphical result of photon transport efficiency. In the individual 3D graph, photon collection is expressed by the photon transport efficiency with respect to the coordinate of the scintillator excitation point. The value of the photon transport efficiency gives the probability that the photon will reach the photocathode of the PMT.

It is evident from the results in Figure 1, that EGS configurations are less efficient than the classical rotationally symmetric ones (see the paper of Schauer and Autrata (1992) for comparison). Of the examined sets of EGS detectors, the most convenient is the one with the circular scintillator and the light guide that widens to a circular profile. It possesses relatively high mean efficiency and the highest homogeneity of efficiency over the scintillator's electron impact surface. Furthermore, it is, like its flange, easy to fabricate. Detectors with strip light guides are inefficient, and detectors with squared scintillators show low homogeneity for the efficiency over the scintillator's electron impact surface.

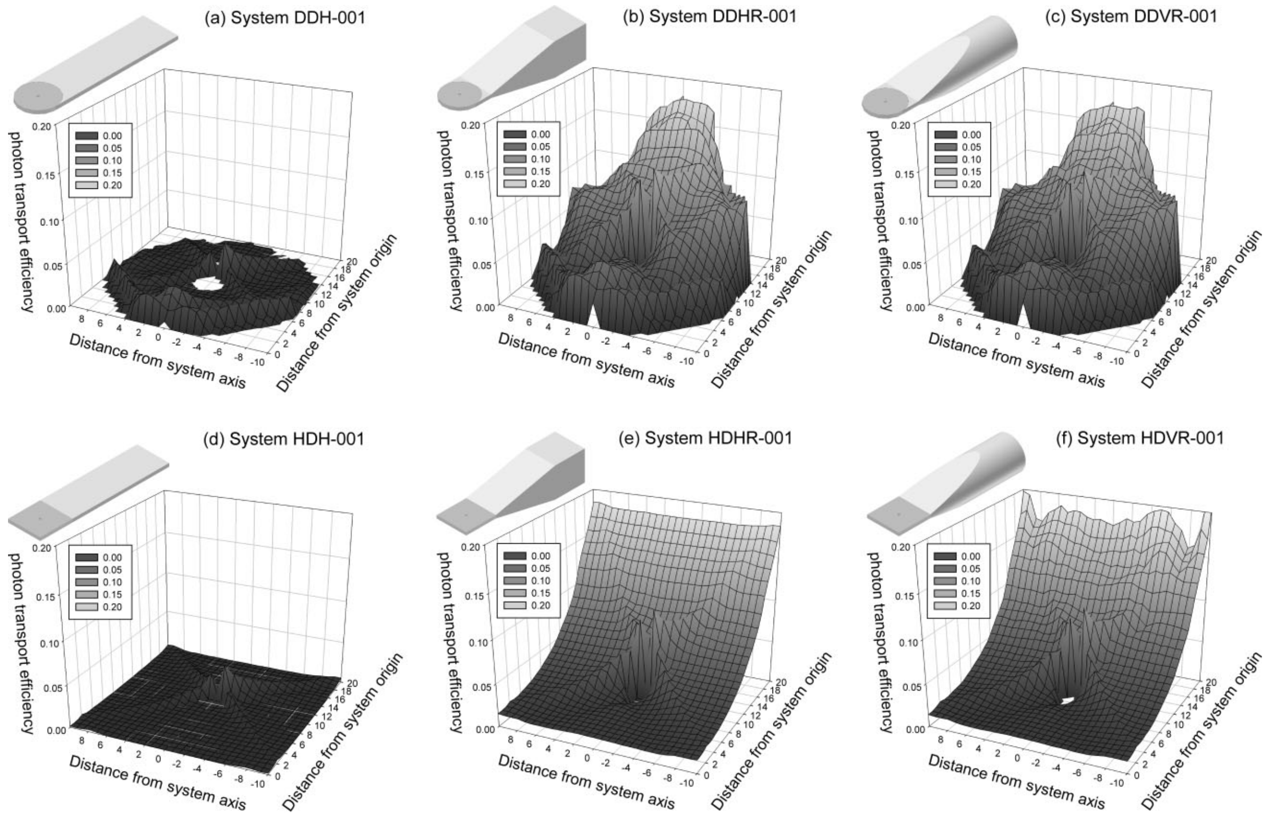

Fig 1. Photon transport efficiency in dependence on the point of excitation on the scintillator surface for different shapes of scintillators and light guides.

The matted scintillator output decreases the efficiency by 15–25%, and therefore it is disadvantageous.

Computer Optimized Design of BSE Scintillation Detector for SEM

The designing of a new BSE scintillation detector for the S 4000 Hitachi SEM was chosen to demonstrate the capability of the introduced MC simulation method. The starting (nonoptimized) detector design was determined by the fixed shape and material of the scintillator, and by the fixed material, length and the output diameter of the light guide (Figures 2a and 3a). A YAG:Ce single crystal disc scintillator (Ø15 × 2.5 mm) with a conical hole (Ø1.5/0.7 mm) and with an indium tin oxide (ITO) coating on the impact surface was used for the EGS detector. The light-guide material was PMMA. The length of the detection system (150 mm) was determined by the distance of electron optical axes from the PMT. The light-guide circular output of 20 mm in diameter was determined by the limited space in the specimen chamber and by the size of the PMT window.

The initial light-guide geometry was determined by the size and by the shape of pole pieces and of the specimen holder. During optimization, only the steps that brought a considerable increase in efficiency were recorded. Geometries and light-guiding efficiencies corresponding to these steps, from the worst (a) to the best (e), are shown in Figures 2, 3, and in Table II. The simulated mean efficiency of the photon transport through the basic configuration (a) was approximately 0.04, as shown in Table II. It is better than the efficiency of the classical ET detector with a disc scintillator (Schauer and Autrata, 1992), and no significant improvement was expected during the detector optimization. But it has been found, that even a small shift of the bottom widening plane to the same coordinate as that for the top plane (Figures 2b and 3b), increases the efficiency to 126%. However, a much greater improvement to 256% has been achieved with geometry (c), after shifting the widening planes as close as the scintillator disc, and after decreasing the angles of the top and the bottom planes to 8° and 14°, respectively. A further improvement to 356% (geometry [d]) has been achieved after configuring the bottom plane so that its slope becomes identical with that of the top plane. The final refinement (geometry [e]) has been accomplished by integrating a conical light-guiding ring (close to the scintillator) into the widening planes of the light guide. The slopes of the planes were only slightly reduced with regard

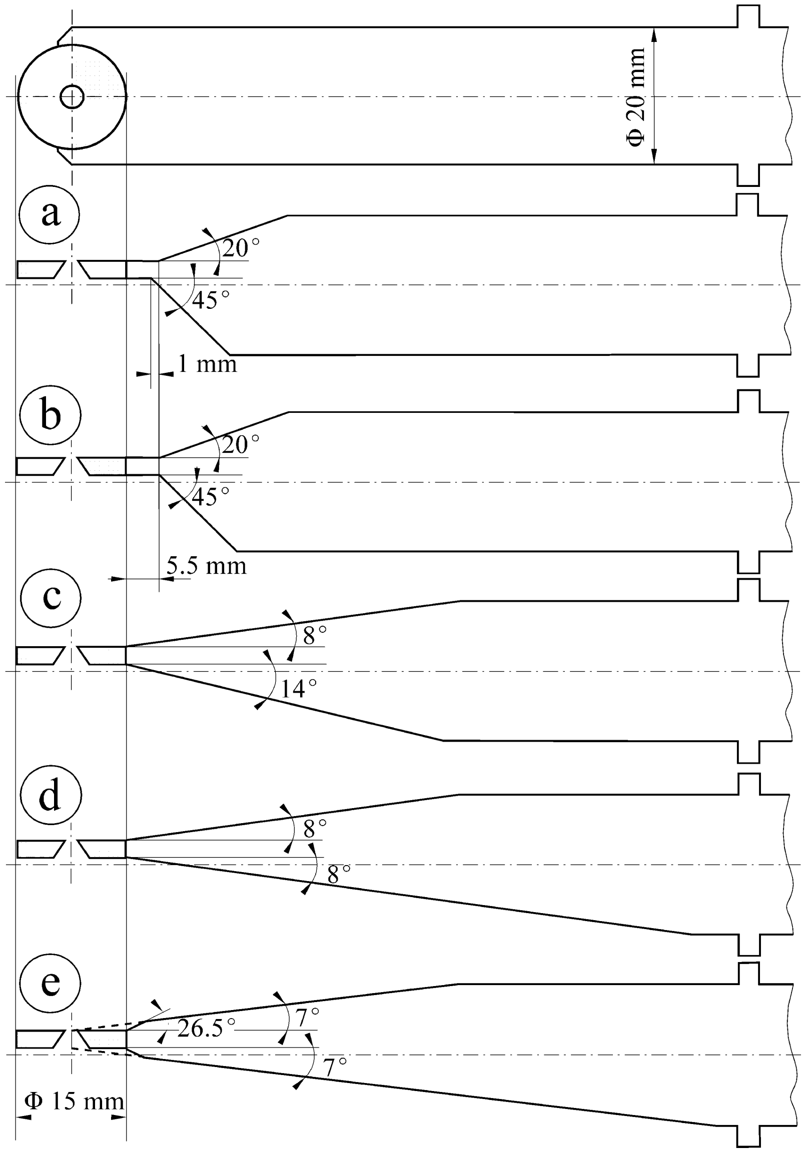

Fig 2. Schematic drawing of the geometry of key configurations during optimization of BSE scintillation detector S 4000 (Hitachi).

to geometry (d). The final light-guiding efficiency is approximately 400% compared with the initial one.

Conclusion

The MC simulation method with the extended algorithm for nearly all shapes of single crystal scintillators and/or of light guides is a very useful tool for the COD of the BSE scintillation detection systems for S(T)EM. Using such a method one can look for some typical relations of EGS BSE detection systems. Furthermore, the described simulation method enables one to design all details of the scintillator and light-guide materials and/or shapes of the particular scintillation detector for a specific SEM vacuum chamber. By applying the

TABLE II. Light-guiding efficiency of the S 4000 BSE scintillation detector in the dependence on different light-guide geometries

Light-guiding geometry[a]	Light-guiding efficiency		
	Mean[b]	Total improvement[c]	Rel. improvement[d]
(a)	0.043	1.00x	—
(b)	0.054	1.26x	1.26x
(c)	0.110	2.56x	2.04x
(d)	0.153	3.56x	1.39x
(e)	0.176	4.09x	1.15x

[a] See Figures 2 and 3.
[b] Over the electron impact surface.
[c] Related to the starting geometry.
[d] Related to the previous geometry.

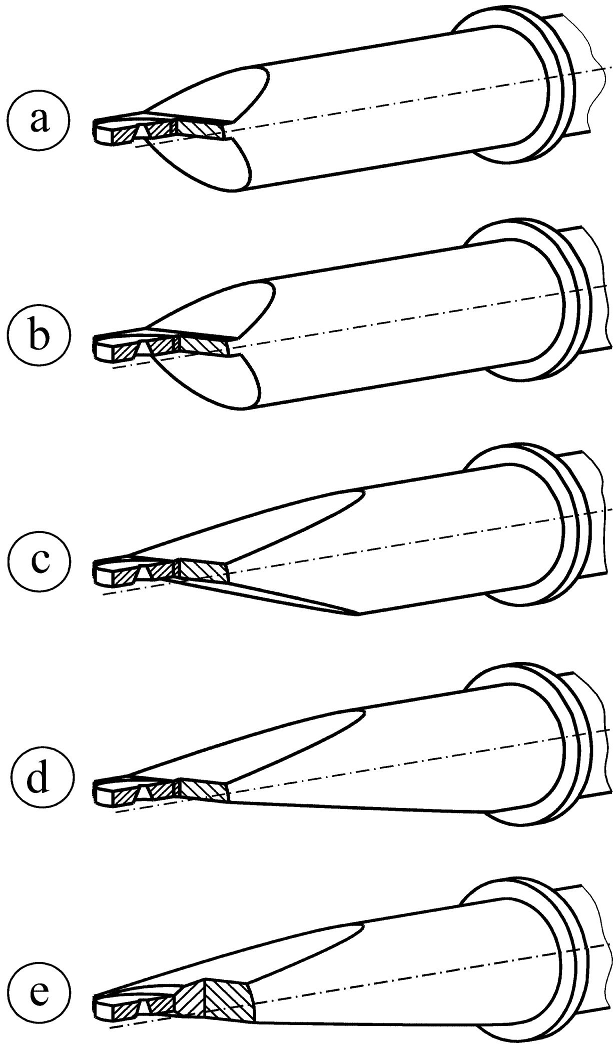

Fig 3. 3D images of the S 4000 BSE scintillation detection systems. Efficiency is improving from the basic (a) geometry to the final (e) geometry.

extended MC simulation method some conclusions can be drawn for EGS scintillation detection systems:

EGS systems are less efficient than classical rotationally symmetric ones. EGS geometries with strip light guides are inefficient. EGS geometries with squared scintillators show low homogeneity of efficiency over the surface of the scintillator. The matted scintillators are inconvenient for EGS systems. The EGS systems with the circular scintillator and with the light guide widening to a circular profile are the most convenient ones. The computer optimized geometry of an EGS scintillation detection system for S(T)EM can increase the final efficiency of the BSE scintillation detector to some hundreds of percent compared with the nonoptimized one.

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