Improved Simulation of the Response Function of Si(Li) detector

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1. Introduction

The detection efficiency and response function of the Si(Li) detector must be determined when it is used in high precision measurements. The detection efficiency of the Si(Li) detector decreases due to the X-ray absorption in the beryllium window, gold electrode, and silicon dead layer for soft X-rays. Distortion of the spectrum due to escape peak and low-energy tailing (tail and flat continuum) is also observed especially below 5 keV [1,2]. The response function remarkably varies depending on the photon energy. A Monte Carlo simulation code was developed for photon energy below 10 keV [3]. Although it gives the physical reason of the tailing for energies below 10 keV, there is a difference in the amount of flat continuum near zero channel. According to the simulation, the gold layer gives main contribution of the flat continuum near zero channel.

In this report, it is shown that a better treatment in the electron scattering processes improves the simulation.

2. Calculation of the response function

Nine possible interactions near detector surface are considered in the simulation as shown in Fig.1. The following processes are considered in the simulation: absorption of incident photons; emissions of photoelectron, Auger electron, and fluorescence X-rays; energy losses of electrons and creation of charge carrier; and charge losses near the detector surface due to surface recombination. The fluorescence X-rays may be absorbed in the detector again and generate the photoelectrons (Auger process is neglected in this case), or escape from the surface which give the escape peak. The ten most intense MNN Auger transitions for M-shell absorption of gold are considered in contrast with the three most transitions in the previous simulation [3].

The photoelectrons and Auger electrons are scattered and lose their energies creating charge carriers along their trajectories in the sensitive volume of silicon. In the previous code, the screened Rutherford (Sc. R) cross section was used to calculate the electron scattering angle and mean free path. However, it is not valid for low energy electrons and high-Z elements. Monte Carlo calculation using the Sc. R cross section shows smaller electron range than experimental values [4]. Therefore more accurate cross section calculated using the partial-wave expansion methods (PWEM)

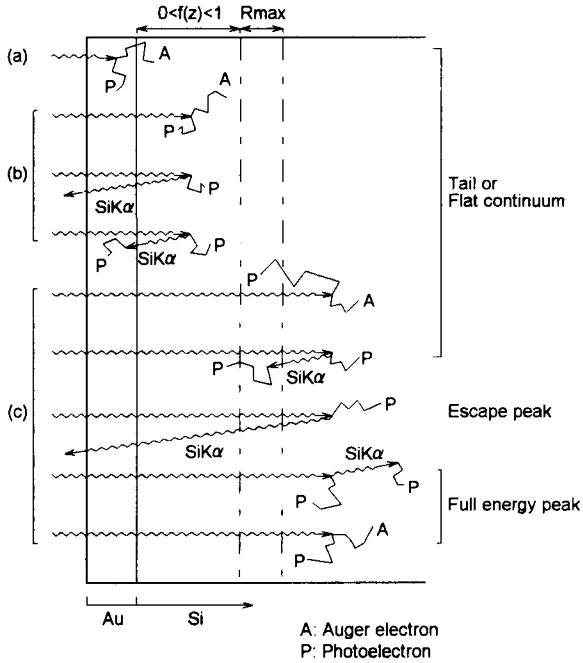

Fig. 1. Interactions of the primary photons, photoelectrons, Auger electrons, and fluorescence near the detector surface. R_{max} is the maximum electron range.

[5,6] is used. The Thomas-Fermi-Dirac potentials are used for silicon and gold atoms. The continuous slowing down approximation (Bethe's formula) is used for the electron energy loss.

To obtain the carrier collection probability as a function of the position where carriers are generated, a simple model was introduced which takes into account drift, diffusion, and reflections due to a finite surface recombination velocity [3]. More detailed treatment of this model is shown here.

The carrier continuity equation is given by

$$\frac{\partial n(z,t)}{\partial t} = -v\frac{\partial n(z,t)}{\partial z} + D\frac{\partial^2 n(z,t)}{\partial z^2}, \qquad (1)$$

with boundary condition and initial condition

$$-D\frac{\partial n(0,t)}{\partial z} + vn(0,t) = -sn(0,t), \qquad (2)$$

$$n(z,0) = \delta(z - z_0), \qquad (3)$$

where n is the carrier (electron) density, z the carrier generation position measured from the gold-silicon interface, t the time after the carrier generation, s the surface (interface) recombination velocity, v a drift velocity, D the effective diffusion coefficient, and z_0 the initial carrier generation position. Solution of carrier continuity equation is given by

$$n(z,t)=\frac{1}{\sqrt{4\pi Dt}}\left[\exp\left\{-\frac{(z-z_0-vt)^2}{4Dt}\right\}\right.$$
$$\left.+\exp\left\{-\frac{(z+z_0-vt)^2}{4Dt}-\frac{vz_0}{D}\right\}\right]$$
$$-\frac{v+2s}{2D}\exp\left\{\frac{(s+v)(z+z_0+st)}{D}-\frac{vz_0}{D}\right\}$$
$$\times\operatorname{erfc}\left\{\frac{z+z_0+(v+2s)t}{2\sqrt{Dt}}\right\}. \qquad (4)$$

Carrier collection probability is calculated by integrating eq. (4) and by taking the limit $t\rightarrow\infty$ as:

$$f(z_0)=\lim_{t\rightarrow\infty}\int_0^\infty n(z,t)dz$$
$$=1-\frac{s}{s+v}\exp\left(-\frac{vz_0}{D}\right). \qquad (5)$$

Infinite surface recombination velocity gives no carrier collection probability at gold-silicon interface. For large z, the carrier collection probability becomes unity. For the case of finite recombination velocity, the probability decreases toward the interface but it does not become zero. The value D/v is estimated to be about 0.1 μm [3]. The values s, v, and D characterize the incomplete charge collection region (dead layer).

For each photon, the fraction of carriers collected by the detector is calculated by summing the product of energy loss in the free path of elastic scattering, $\Delta E(z)$, and the carrier collection probability, $f(z)$, along the electron trajectories. The collected carrier number is given by

$$N=\sum_j\sum_i\frac{\Delta E_i(z)}{\varepsilon}f(z) \qquad (6)$$

where, ε is the mean energy to create electron-hole pair, i the step of electron scattering, and j electron energy loss processes. By simulating the carrier number for each photon using a Monte Carlo method, the response function is calculated.

3. Results and discussion

Figure 2 shows calculated and measured response functions for 6-keV photons. Details of the measurement are shown in ref. [3]. Good agreement of flat continuum using the cross section by PWEM is clearly demonstrated. Figure 3 shows tail-to-peak ratio as a function of the photon energy. Figure 4 is the ratio of counted photons after absorption in the gold layer (C_{Au}) to the total photons counted as the response function (C_{total}). The discrepancy between measurements and previous calculations (Sc. R) is explained to be due to the underestimation of electron range.

The integrated detection efficiency (full energy peak and the low-energy tailing) is almost identical with the transmittance in the front gold layer showing the maximum difference of 2% at Au M_4 absorption edge. It describes well the experimental results of Scholze et al. [2].

References

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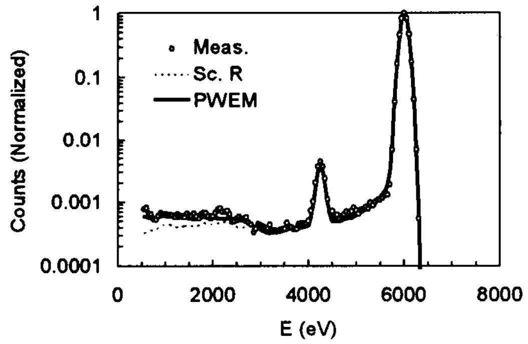

Fig. 2. Response function for 6-keV photons. 20-nm-thick Au layer is assumed. D/v= 0.09 μm and $v/(s+v)$= 0.45.

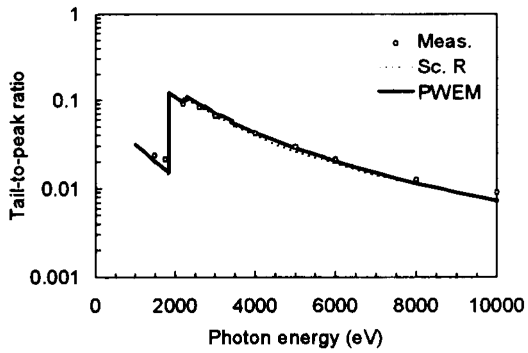

Fig. 3. Tail-to-peak ratio.

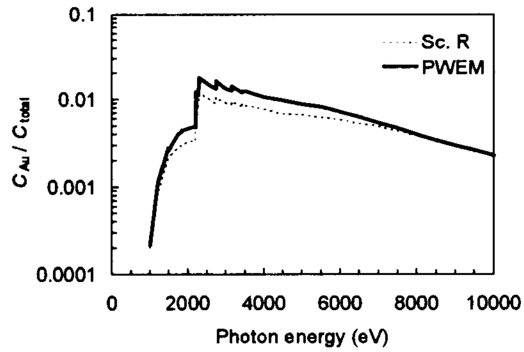

Fig. 4. Contribution of gold layer to the response.