Systematic errors that depend on diffusivity and absorptance of sample in IEC method for absolute photoluminescence quantum efficiency

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Photoluminescence quantum efficiency is one of the important parameters for lightings and display industries characterize when photoluminescence materials. An IEC paper provides well organized method for absolute photoluminescent quantum efficiency [1]. However, its systematic errors that can occur in specific conditions, in where some of their assumptions are not valid, has not been studied. In this paper, we studied systematic error with Monte-Carlo ray-tracing simulation. From this calculation, we showed that systematic error of the method depends on diffusivity IEC and absorptance of sample under the test. The highest systematic error exhibits 17% with diffuse reflective sample.

INTRODUCTION

The phtoluminescent (PL) materials like as quantum dots have been one of important the materials for lightings and display industries. In these fields, PL measurement has been important tool to study bandgap structure of PL materials. However, this qualitative sudy is not enough for applications to characterize the PL materials. The quantitative PL measurement such as PL quantum efficiency (PLQE) have been started to be crucial for display and lighting applications [2].

For the measurement of PLQE, goniometric method and integrating sphere based method were developed and widely have been used. The goniometric method can measure an angular distribution as well as the total photon flux of PL emission. However, it is very slow compared to the integrating sphere method.

Otherwise, the integrating sphere method is speedy compare to the goniometric method [3]. One of the methods widely used, named as 'collimated incident light method (CILM)', has been developed by J. C. Mello et al, and chosen as IEC standard (IEC62607-3-1) [1,4]. This method was designed to compensate the effects where affect on result of PLQE measurement, such as reabsorption of sample and spectrally non-neutral reflectance of sphere wall. However, it still contains few assumptions that can cause systematic errors, like as specular reflection (zero-diffusivity) of the sample and zero-absorption of the sample in PL emission wavelength ($A_{emit} = 0$).

In this paper, we investigated the CILM in numerical way with a Monte-Carlo ray-tracing simulation tool (software: RayWiz¹). We figured out that maximum systematic error was 17% in particular condition.

SIMULATION METHOD AND RESULTS

Based on the CILM, we conduct simulation using ray-tracing software to evaluate the systematic errors asrising from the assumptions mentioned before. In this numerical experiement, we assigned the value of PLQE, then, performed virtual experiment based on CILM. The systematic error was evaluated with comparison between the values of PLQE assigned (η_a) and PLQE virtually measured (η_m) . Figure 1 shows 3D image of numerical experimental setup.

The virtual experimental setup has been built complying conditions presented in the IEC paper, such as integrating diameter, port size and positions of baffles. We set the number of excitation rays for simulation set to 2×10^7 .

The integrating sphere is set to exhibit diffusive reflection ($D_s = 1$, Lambertian reflection), and reflectance of the sphere is spectrally neutral. The



Figure 1. 3D image of numerical experimental setup



Figure 2. Relative error when $D_s = 1$



Figure 3. Relative error with respect to A_{PL}

diameter of the sphere inside and sample was set to 150 mm, and 15 mm. The dimensions for simulation are shown in Fig. 1.

Figure 2 shows calculated relative error $\varepsilon = (\eta_m - \eta_a)/\eta_a$ [%] when the virtual sample is set to exhibit diffusive reflection ($D_s = 1$). Reflectance of the sampe at excitation wavelength (A_{exc}) was set to 0.6, and $A_{PL} = 0$. The relative error for each reflectance (0.95, 0.97, 0.99) is evaluated to 17%, 8%, and 2%, resepctively.

The relative error in virtual experiment with respect to A_{emit} is shown in figure 3. A_{exc} , η_a is set to 0.6 and 0.9, respectively. These values are arbitraly chosen, because they do not affect on the result. The largest relative error was evaluated to 10% in minus when $A_{PL} = 0.8$.

CONCLUSION

This work has investigated systematic errors in the IEC standard method for PLQE measurement of PL

materials through numerical experiments using a commercial ray-tracing software. It is found that the underlying assumption of the IEC method causes an error of 17% at most when a diffuse relective sample is measured using an integrating sphere of 0.95 reflectance. Futhermore, non-zero A_{PL} cause error of 10% in minus when A_{PL} was 0.8.

We also developed a method for compensation of the systematic errors, and presented in a paper [5]. Two more experimental steps with auxiliary light at PL emission wavelength is added for the compensation. We also tested this method with numerical experiments, then, we found that the systematic errors were succesfully suppressed with the compensation method.

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