Computational analysis of the emission of ZnO nanowires and coreshell CdSe/ZnS quantum dots deposited on different substrates

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INTRODUCTION

Core-shell type quantum dots have received much attention due to their ability to improve the photoluminescence quantum yields by passivating surface nonradiative recombination sites [1]. These quantum dots, nanowires and nanostructures have been extensively studied due to their unique optical properties. Zinc oxide (ZnO) nanowires have also been of great interest together with other 1D-nanostructures, such as semiconducting nanowires [2], carbon nanotubes [3] and nanobelts [4] due to their potential multifunctional applications due to their optoelectronics and piezoelectric properties [5]. In this study, we have investigated the computational analysis of the scattered field from four different substrates such as gallium arsenide (GaAs), silicon (Si), glass and indium tin oxide (ITO) to investigate the effects of the substrates on the photoluminescence (PL) emission spectra of CdSe/ZnS core-shell quantum dots (QD) and as grown ZnO nanowires (NWs).

RESULTS AND DISCUSSIONS

To investigate the effects of substrates on the emission spectra of quantum dots and ZnO nanowires, we used FEKO Lite software. This computational analysis was carried out to see the influence of scattering of the incident field from the surface of different substrates. Figure 1 shows the schematic diagram of the structure used for simulation which is a square shape structure in exposure of Z-directed uniform incident plane wave (black arrow). The incident plane wave is of single frequency wave with a wavelength of 325 nm. Figure 2 and 3 shows the Poynting vector of the scattered field and the total field versus the position from the surface of substrate. The scattering wave can be thought as the reflection from all angles while reflection coefficient of a normal polarized and a parallel polarized plane waves can be expressed as shown in equation 1 and 2.

$$\Gamma_{\perp} = \frac{\cos\theta i - \sqrt{(\varepsilon_{2r}/\varepsilon_{1r}) - \sin^2\theta i}}{\cos\theta i + \sqrt{(\varepsilon_{2r}/\varepsilon_{1r}) - \sin^2\theta i}} \quad (1)$$

$$\Gamma_{\parallel} = \frac{-\cos\theta i + (\varepsilon_{1r}/\varepsilon_{2r})\sqrt{(\varepsilon_{2r}/\varepsilon_{1r}) - \sin^2\theta i}}{\cos\theta i + (\varepsilon_{1r}/\varepsilon_{2r})\sqrt{(\varepsilon_{2r}/\varepsilon_{1r}) - \sin^2\theta i}} \quad (2)$$

where the θi is the incident angle. The Poynting vector is the directional energy flux density from the substrate and can be expressed as following:

$$\bar{P} = \bar{E} \times \bar{H} \quad (3)$$

As shown in Fig. 2, the value of the Poynting vector of the scattered field from the surface of GaAs has the maximum value while glass has the least. Comparing with the experiment results shown in Figure 4 and the simulation results in Figure 5, it can be seen that the PL intensity of the quantum dots from each substrate is dependent on the scattering field from the surface of substrate. In the case of ITO-coated glass, metals cause absorption loss into the cavity [7]. Hence, the emission intensity of quantum dot and ZnO NWs deposited on the ITO-coated glass is even lower than from the glass substrate. The comparisons of simulation results shown in Fig. 2 and Fig. 3 demonstrate that the value of scattered field at the surface determines the emission intensity from a particular substrate rather than the total field or the different types of deposited material.

CONCLUSIONS

We investigated origin of the differences of emission intensities of CdSe/ZnS quantum dots and as grown ZnO NWs deposited on GaAs, Si, Glass and ITO-coated glass using computational Poynting vector simulations. The simulation shows that the substrates having the maximum scattered field has the strongest PL emission intensity and is independent of the whether quantum dots or ZnO nanowires were used.

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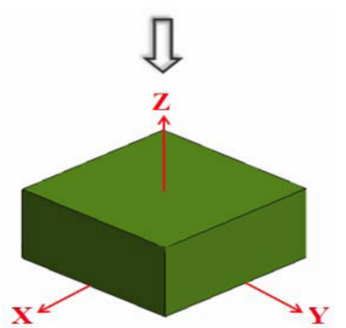

Fig. 1. Schematic diagram of structure used in simulation

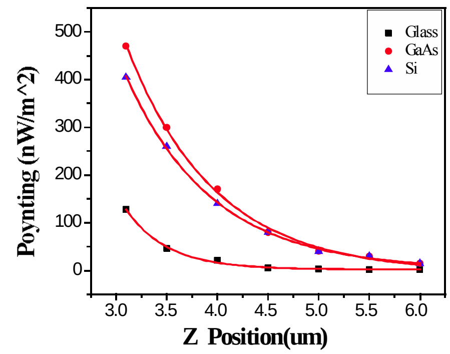

Fig. 2 Poynting vector of scattered field versus z-position distance from the surface of substrate.

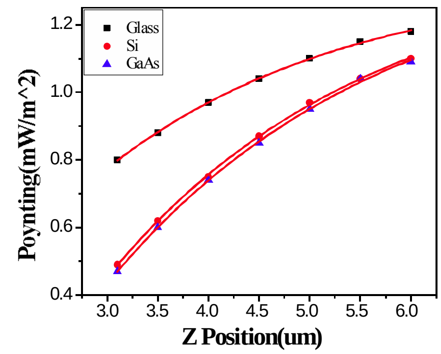

Fig. 3. Poynting vector of total field versus position from the surface of substrates.

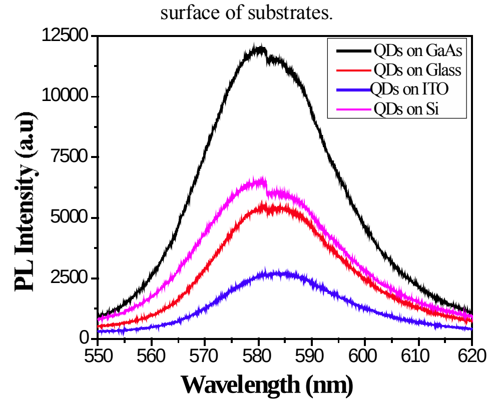

Fig. 4. Photoluminescence spectra of CdSe/ZnS quantum dots on different substrates

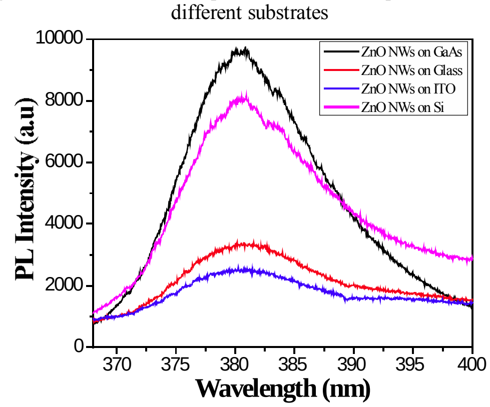

Fig. 5. Photoluminescence spectra of ZnO nanowires on different substrates