High Accuracy Quantum Dots (QDs) Simulation Model for Color-Conversion Micro-LED Display

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Abstract

We have successfully established a high accuracy quantum dots(QDs) simulation model to be actively adaptable against QDs layer input parameters varieties through LightTools; Input Parameters (i) QDs Layer thickness, (ii) QDs concentration and (iii) TiO2 concentration. By applying a uniquely-determined calibration factor that relates to distance between QDs, simulation accuracy drastically improved to practical level. Our new high accuracy QDs model is useful to precisely predict conversion efficiencies of the QDs layer and explore the optimized structure for practical QDs applications, mainly Color Conversion Micro-LED display.

Author Keywords

Quantum Dots (QDs), simulation accuracy, optical modeling, ray tracking, Color Conversion Micro-LED display

1. Introduction

The Micro-LED display, which has a long lifetime and high luminous efficiency, can be expected to become the mainstream of the next-generation display technology. However, there are many challenges such as transferring for three kinds of chips made through three different epitaxial growth processes and driving complexities. One effective approach to avoid the mass-transferring of three different kinds of chips is GaN-based Micro-LED structure combining with QDs layer. To precisely predict the efficiency of Color Conversion Micro-LED (CC Miro-LED) display, high accuracy QDs simulation model is essential to be actively-adaptable against various QDs input parameters such as QDs layer thickness, QDs and TiO2 concentration.

Previously, optical trends in performance such as unconverted light output (blue transmission) and green converted light output, which have been investigated in various QDs input parameters of QDs layer through LitghtTools (LT) [1,2]. However, the comparison between experiment/simulation, as well as simulation accuracy has not been described at all.

An another report shows an optical modeling based on mean free path calculations for application of QDs-based white LED and OLED displays by LT [3]. Although the QDs model has good agreement between experiment/simulation in terms of color and normalized PL spectrum, the simulation result does not include quantitative output values regarding unconverted / converted light of the QDs layer. Moreover, since the optical model does not have any scattering particles (i.e. TiO2), it is not suitable to explore the optimized structure for practical CC Micro-LED display requiring high blue absorption.

Also, a further another report shows that FDTD (Finite-Difference Time Domain) was performed for revealing the light-enhancement mechanisms on QDs embedded in anodic aluminum nano-structure [4]. However, FDTD may have better accuracy at smaller than ~10λ, while at larger than ~10λ, enormous amount of resources that include the computing power and time should be required, thus being not good method for predicting the conversion efficiency of QDs layer.

Table1. Pros / Cons regarding two representative optical simulation software

	LightTools (LT)	FDTD
Method	Based on Geometrical optics (Ray Tracking)	Based on Wave optics (Maxwell's equations)
Pros	For > ~10λ, accuracy is better	For < ~10λ, accuracy is better
Cons	For < ~10λ, accuracy is worse due to not-considered wave optics	For > ~10λ, enormous amount of computing power / time is required

Although pros / cons regarding these two software have been shown in Table1, both have difficulty in precisely predicting the conversion efficiency of QDs layer with quick time.

In this paper, we have proposed a high accuracy QDs simulation model to be actively adaptable against QDs layer input parameters varieties through LT; Input Parameters (i) QDs layer thickness, (ii) QDs concentration and (iii) TiO2 concentration. By applying a uniquely-determined calibration factor (cf) that relates to distance between QDs, simulation accuracy drastically improved to practical level. Our new high accuracy QDs model is useful to precisely predict the conversion efficiency of the QDs layer and explore the optimized structure for practical CC Micro-LED.

In Fig.1, QD collision modes has been shown as three cases. First is no collision mode, which shows the blue transmitted. Second is blue scattering mode by QDs having high refractive index (n~4@λ460nm). Third is mode which converts excitation blue light to red luminescence. In short, these three cases are functionally-supported by LT, while optical interaction between QDs when excitation light collides with QDs, is not supported due to wave optics phenomenon. Where, cf needs to compensate for no-support function. QDs concentration is high enough to put into practical CC Micro-LED display (i.e. distance between QDs is

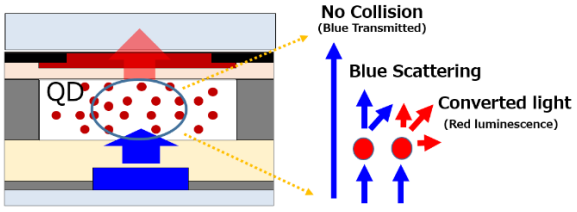

Figure 1. Schematic of 3 cases of collision between QDs and blue excitation lights (Red Scenario)

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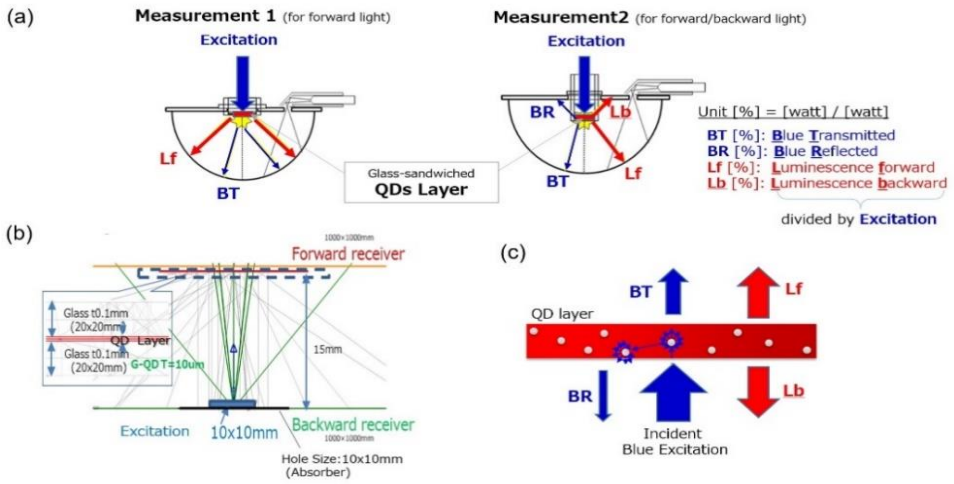


Figure 2. Evaluation of optical properties of QDs Layer (a) Experiment system, (b) Simulation model configure and (c) 4 indicators(B_T, B_R, L_f, L_b) when blue excitation enters into QDs layer

too short), the accuracy simulated by LT may be predicted to be worse.

2. Methods

Figure2 shows the experiment system and defined simulation components for obtaining forward / backward light output of QDs layer when blue excitation light enters. For precise measurement, the QDs layer was composed of being sandwiched by a pair of glass to prevent QDs from degrading due to oxygen and moisture. The QDs layer consists of three components, which are InP-based QDs, TiO2 and Polymer binder.

As shown in Fig.2(a), optical measurement has been conducted by two steps using a quantum efficiency measurement system (QE2100, Otsuka Electronics) ; one step is that measurement1 known as forward light mode, was utilized for obtaining forward light components, which means blue transmission (B_T) and luminescence forward (L_f). Another step is that measurement2 was utilized for obtaining "forward + backward light" components. By subtracting energy output of mesurement1 from that of measurement2, blue reflection (B_R), luminescence backward (L_b) was extracted, respectively.

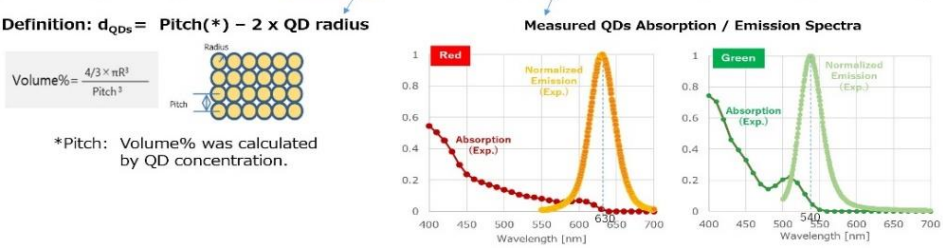
In Fig.2 (b), simulation model was configured by LT (Version 2022.03) that is known as ray tracking simulation software. The model, analogous to experiment system, consists of three distinct elements; glass-sandwiched QDs layer, a blue excitation light source that is collimated at wavelength of 460nm, and forward / backward receivers that can detect unconverted / converted lights from the QDs layer. Figure2 (c) shows the schematic 4 indicators (B_T / B_R / L_f / L_b) in QDs layer model, when blue excitation enters into layer. These four indicators are used to compare experiment with simulation.

(Simulation parameters for InP-based QDs model)

Table 2 shows our simulation parameters for Red / Green InP-based QDs. In conventional QDs model, QDs measurable optical properties (i.e. PLQY~90%, absorption / emission spectra) have been important as input parameters. A wavelength dependent mean free path (MFP (λ)), which was auto-calculated based on both QDs concentration (i.e. distance between QDs; $\mathbf{d_{QDs}}$) as well as QD cross-sectional areas (calculated by QD material sizes / refractive index). Also, QDs self-absorption was functioned under ray-tracking simulation as a loss in stokes shift, in order to improve the accuracy. TiO2, which behaved as a blue scattering particle to increase absorption of excitation in the QDs layer, were input in measured values (i.e. particle radius ~ 130nm / refractive index ~2.4). In contrast, our new QDs model has a uniquely-determined calibration factor (cf) that was added newly to conventional QDs model. The cf has been an extremely key component of one of QDs input parameters, and depended mainly

Table 2. Simulation parameters for Red / Green InP-based ODs

		QD simulation parameters						
Color	QD Model	QDs Layer Thickness	MFP(λ)	calibration factor	Distance btw QDs (d_{QDs})	Absorption / Emission Spectra	Quantum yield: PLQY (B460)	Quantum yield: Self-Absorption
Red	Conventional	10~20um	1.9um (B460)	No Valid	6.3 ~ 27nm	Measurement (Scale Factor calculated)	Measurement	Stokes Shift
	New			Valid				
Green	Conventional	↑	1.3um (B460)	No Valid	4.0 ~ 20nm	↑	↑	↑
	New			Valid				
		Variable Parameter	Auto-Calculated	Key Input	Variable Parameter	Input	Input	Auto-calculated



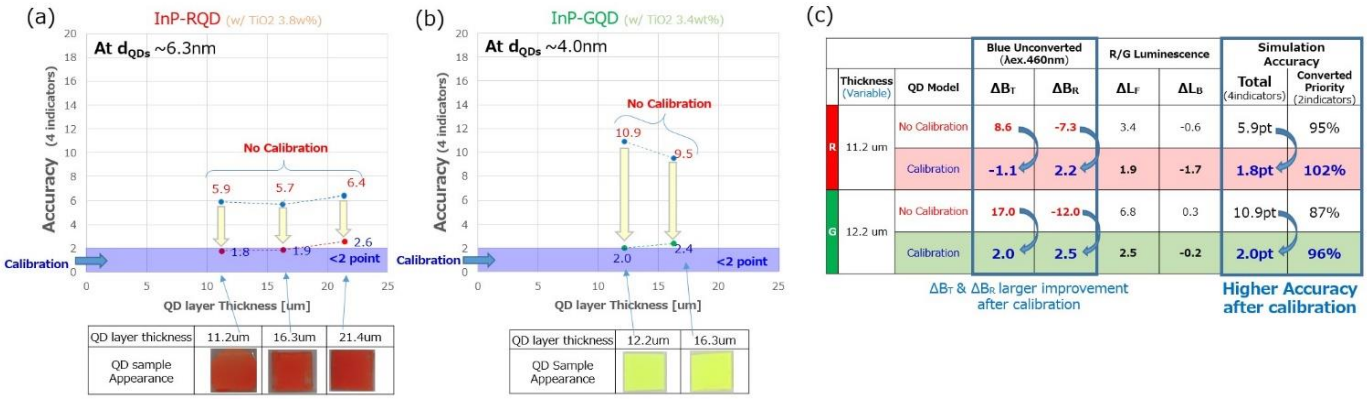


Figure3. Simulation accuracy v.s. QDs thickness (a) R-QDs, (b) GQDs, (c) Each differences against 4indicators

on both QDs and TiO2 concentration.

3. Results and Discussion

As a first validation of QDs model simulation accuracy, optical properties (ratio of unconverted and converted light to incident blue energy) of three different QDs layers at fixed d_{QDs} (Red ~6.3nm / Green~4.0nm) were measured in layer thickness range from 10 ~ 20um. Then, total accuracy towards QDs layer, was defined as an equation (1) that is based on 4 indicators below;

$$\text{Total Accuracy[pt]} = \sqrt{\left(\Delta B_T^2 + \Delta B_R^2 + \Delta L_f^2 + \Delta L_b^2\right)/4} \cdots (1)$$

$$\Delta B_n = B_n(experiment) - B_n(simulation) \quad \text{(n: T, R)}$$

$$\Delta L_m = L_m(experiment) - L_m(simulation) \quad \text{(m: f, b)}$$

Where, above accuracy has been interpreted as average deviation from experimental values against all the unconverted / converted lights. In addition, focusing on forward/backward converted lights out of 4 indicators, accuracy defined by average ratio of simulation /experiment was defined as an equation (2);

$$\text{Conveted lights prioritized Accuracy[pt]} = \left(L_{f\ (sim)}/L_{f(\text{exp})} + L_{b\ (sim)}/L_{b(exp)}\right)/2 \cdots (2)$$

(i) Variable Parameters: QDs Layer thickness

Figure3 shows the simulation accuracy versus different QDs layer thickness (10~20um), which was fixed at d_{QDs} (R6.3nm / G4.0nm) and fixed TiO2 concentration (~4wt%).

In Fig.3 (a), in conventional model (no calibration), the accuracy indicated a poor value of ~6point due to not-considered wave optics between QDs. In contrast, in new model (calibration), the accuracy drastically improved up to 2point. This means our QDs model was actively adaptable in thickness range up to ~ 20um.

In Fig.3 (b), green InP-QDs also gained same level of accuracy regardless of TiO2 concentration. Also in different thick QDs layers without TiO2, these accuracies improved from >10point (no calibration) to 2point (calibration). Therefore, introducing cf that uniquely relates to distance between QDs, which can lead to the realization of high accuracy QDs model to be actively adaptable against different layer thickness.

As one of reasons that our QDs model has high accuracy, in Fig3. (c), especially ΔB_T, ΔB_R out of 4 indicators drastically improved after calibration. The possible reason is that, blue unconverted light that has shorter wavelength, which has been susceptible to wave optical interaction between QDs. Importantly, total accuracies have strong relation with converted-light-prioritized accuracy, which has substantiated the validity against aforementioned definition on total accuracy.

(ii) Variable Parameters: QDs concentration

Figure4 shows the simulation accuracy versus distance between QDs (d_{QDs}; R 6.3~27nm / G 4.0~19.6nm), which was fixed at QDs layer thickness (~10um). The distance between QDs (d_{QDs}) have corresponded to QDs conc. range requested in QDs applications.

For constructing cf database for $\mathbf{d_{QD}}$ varieties, conversion efficiencies of QDs layer were measured through QE2100 by changing QDs concentration at fixed high TiO2 conc.(~4wt%).

In Fig.4 (a), in conventional model (no calibration), the accuracy was relatively low when $\mathbf{d_{QDs}}$ was smaller than 20nm. Specifically, before calibration, accuracies at different $\mathbf{d_{QDs}}$

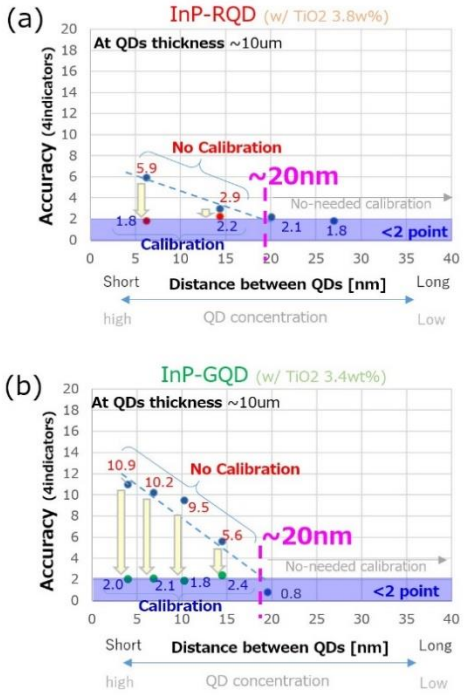


Figure 4. Simulation accuracy v.s. d_{QD} (a) R-QDs, (b) G-QDs

6.3/14.4nm have shown low value as 5.9/2.9point, respectively. After calibration, these accuracies improved to be good as 2.0point. Meanwhile, if $\mathbf{d_{QDs}}$ was longer than ~20nm, the accuracy kept high even without calibration. The possible reason is that such a longer $\mathbf{d_{QD}}$ is not needed due to weaker wave optical interaction between QDs, compared to < 20nm.

In Fig.4 (b), green InP based QDs also gained same level of accuracy with calibration when $\mathbf{d_{QDs}}$ is smaller than ~20nm. Where, green InP based QDs have higher QDs concentration than red ones, thus stronger calibration can be needed due to stronger optical interaction between QDs. In different QDs concentration without TiO2, these accuracies improved to 2point.

Judging from validated results above, we have importantly found out the fact that cf has been expressed as an approximate equation below;

$$\mathbf{cf} := \mathbf{cf}\,(\mathbf{QDs\ conc.}, \mathbf{TiO2\ conc.}) \propto A * exp^{-B*d_{QDs}}$$

Where, A, B is constant to be decided uniquely by QD physical property. To the point, cf is the key input parameter based on Mie theory, where wave optical interaction between QDs can be considered to compensate for LT no-supported function. That's why our QDs simulation model also has been theoretically substantiated.

As a conclusion, by introducing cf that relates to $\mathbf{d_{QDs}}$, into QD model, simulation accuracies improved to ~2points. It is proved that our QDs simulation model has been actively-adaptable against different QDs concentration, especially also even high QDs conc. required in CC Micro-LED.

(iii) Variable Parameters: TiO2 concentration

Figure 5 shows the simulation accuracy versus different TiO2 concentration (~4wt%), which is fixed at both QDs thickness (~10um) and d_{QDs} (R6.3nm or G4.1nm). For accuracy validation against TiO2 concentration, cf at fixed QDs concentration was defined by a simplified equation below;

$$\mathbf{cf}\,(\mathbf{TiO2\ conc.}) = \mathbf{cf}\,(\mathbf{High\ TiO2\ conc.}) \times \boldsymbol{\alpha} + \mathbf{cf}(\mathbf{Low\ TiO2\ conc.}) \times (\mathbf{1} - \boldsymbol{\alpha})$$

Where, α is TiO2 concentration coefficient. α=0 corresponds to low TiO2 concentration, and α=1 is equal to high TiO2 concentration. Here, α=0.5 means TiO2 middle concentration, then cf was calculated as weighted average value in between high/low TiO2 concentration.

By applying calculated cf above into QDs model, simulation accuracy improved to ~2point compared to no calibration (Fig.5 (a), (b)). This means our QDs model is actively adaptable against TiO2 concentration (~ 4wt%). In Fig4. (c), especially ΔB_T, ΔB_R out of 4 indicators drastically improved. Besides these three cases, TiO2 concentration range in 0<α<1 can be also predicted for having high accuracy.Therefore, introducing the cf that uniquely relates to distance between QDs can lead to the realization of high accuracy QDs model to be actively adaptable even against different TiO2 concentration.

4. Impact

We have successfully enabled a high accuracy InP-based QDs simulation model to be actively adaptable against QDs layer input parameters through LightTools; Parameters (i) QDs layer thickness, (ii) QDs concentration, (iii) TiO2 concentration.

By applying our original uniquely-determined calibration factor that relates to distance between QDs($\mathbf{d_{QDs}}$), simulation accuracy drastically improved to ~2point in layer thickness range up to ~20um, which these values have advantage of easier fabrication. Also in terms of QDs concentration varieties, the accuracy improved to ~2point in $\mathbf{d_{QDs}}$ range all from 4 to ~30nm. This mean our new QDs model has high accuracy and is also actively adaptable against different QDs concentration, where even high QDs concentration included. Finally, our QDs model has high accuracy as well against different TiO2 concentration.

Our new QDs simulation modeling method can be applied towards Perovskite nanocrystals, which have some advantages such as high PLQY and high blue absorption compared to InP based QDs. Plus, new high accuracy QDs model is useful to precisely predict the conversion efficiencies of the QDs layer and explore the optimized structure for practical QDs applications, i.e. QD-OLED, QD-LCD and mainly CC Micro-LED display.

5. References

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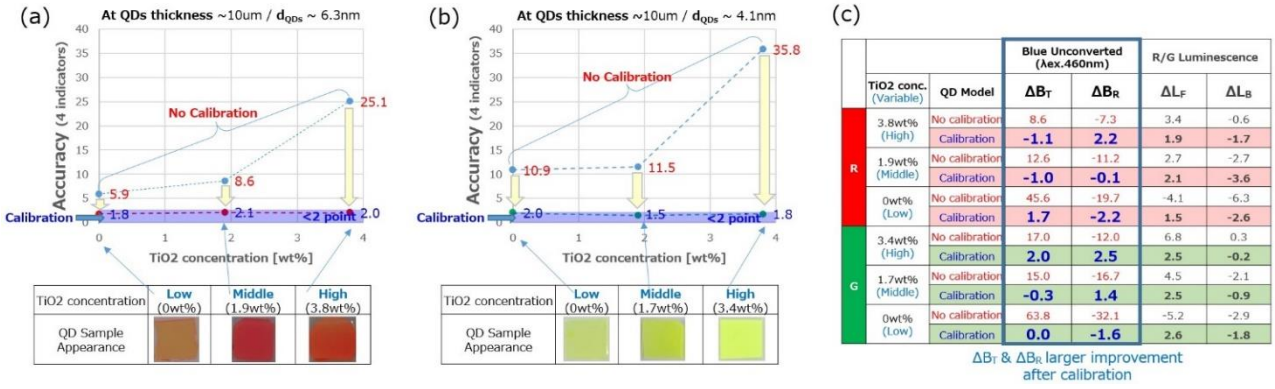

	TiO2 conc. (Variable)	QD Model	Blue Unconverted (λex.460nm) ΔB_T	ΔB_R	R/G Luminescence ΔL_F	ΔL_B
R	3.8wt% (High)	No calibration	8.6	-7.3	3.4	-0.6
		Calibration	-1.1	2.2	1.9	-1.7
	1.9wt% (Middle)	No calibration	12.6	-11.2	2.7	-2.7
		Calibration	-1.0	-0.1	2.1	-3.6
	0wt% (Low)	No calibration	45.6	-19.7	-4.1	-6.3
		Calibration	1.7	-2.2	1.5	-2.6
G	3.4wt% (High)	No calibration	17.0	-12.0	6.8	0.3
		Calibration	2.0	2.5	2.5	-0.2
	1.7wt% (Middle)	No calibration	15.0	-16.7	4.5	-2.1
		Calibration	-0.3	1.4	2.5	-0.9
	0wt% (Low)	No calibration	63.8	-32.1	-5.2	-2.9
		Calibration	0.0	-1.6	2.6	-1.8

ΔB_T & ΔB_R larger improvement after calibration

Figure5. Simulation accuracy v.s. TiO2 concentration (a) R-QDs, (b) G-QDs, (c) Each differences against indicators