

Effect of V-shaped pit density on quantum efficiency of blue InGaN/GaN multiple-quantum well light-emitting diodes: Simulation

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Abstract

LEDs with different density of V-shaped pits are numerically investigated. To validate the used models and parameters, the experimentally external quantum efficiency (EQE) curve of blue InGaN/GaN multiple quantum well light-emitting diode (LED) is fitted with the calculated EQE curve. Simulation results show that the EQE is firstly enhanced and then reduced with an increase in the density of pits. The optimal value of the density is about $2.5e9 \text{ cm}^{-2}$.

I. INTRODUCTION

GaN-based light-emitting diodes (LEDs) are of great interest for applications in lighting, displays, biotechnology, sensing, medical instrumentation, and other areas [1]. However, there is a high density of threading dislocations (TDs) ($10^8 \sim 10^{10} \text{ cm}^{-2}$) in InGaN/GaN LED grown on foreign substrates, due to the poor matching between the epi-layer and substrate in the lattice parameter and the thermal expansion coefficient. In spite of being non-radiative recombination centers [2], the TDs can be self-screened by the formation of V-shaped pits, induced from dislocations, with six {10-11}-oriented sidewalls [3-6]. In addition, due to the lower polarization charge densities in the sidewall structure with lower In concentration and {10-11}-oriented semi-polar facets, the injection of holes into the MQW via the sidewalls of the V-shaped pits is easier than via the flat region [7]. Therefore, InGaN-based LEDs with high dislocation density still have high emission efficiency. A lot of research is focused on the role of V-shaped pits screening the dislocations, but the effect of V-shaped pits on hole injection has only recently begun to get attention [7, 8]. It is found that the V-shaped pits has a significant influence on the hole injection depth [8]. In our previous work [7], a physical model about hole injection enhanced by the V-shaped pits has been established by using numerical simulation. According to this model, the hole injection can be sharply improved by increasing the number of pits. So the density of V-shaped pits has a marked impact on quantum efficiency (QE) of LED. Hence, it is important to optimize the density of pits for improving the performance of LED.

In this paper, the LED structure is carefully designed for the density of V-shaped pits. The effect of the V-shaped pits

density on the quantum efficiency of LED is predicted quantitatively. The optimal value of the density is obtained.

II. DEVICE STRUCTURE AND SIMULATION MODELS

To validate the used models and parameters, the experimentally external quantum efficiency (EQE) curve is fitted with the calculated EQE curve. Reference sample was grown on silicon (111) substrates by Thomas Swan close-coupled showerhead (CCS) metalorganic chemical vapor deposition (MOCVD) reactor. An AlN buffer layer is deposited on a Si substrate at first, then a Si-doped ($3e18 \text{ cm}^{-3}$) n-type GaN with a thickness of $2.5 \mu\text{m}$ is grown on the top of the buffer layer, and followed by a Si-doped-InGaN/GaN short period SL structure. The SL structure, grown at a low temperature and slow growth rate, is pits generation layer, and consists of dozens of periods of InGaN well layers and GaN barrier layers. Nine periods of InGaN(3nm)/GaN(10 nm) MQW active regions is grown on SL structure, followed by a 30-nm-thick Mg-doped GaN hole injection layer (HIL), a 20-nm-thick Mg-doped AlGaIn electron blocking layer (EBL), and a 80-nm-thick Mg-doped GaN cap layer. Schematic epitaxial structure with V-shaped pit for the experimental sample is shown in the inset of Fig. 1. Details of the growth can be found elsewhere [9]. Vertical structure LED chips of $1\text{mm} \times 1\text{mm}$ were fabricated with the n-GaN up and roughened surface. The detailed chip fabrication process has been reported [10]. The EL test system contains the CAS140CT spectrometer and the integrating sphere made by Instrument Systems, and 2635A Sourcemeter made by Keithley Instruments, Inc.

The software used for numerical simulation is the ATLAS program, which was developed by SILVACO Inc. The primarily physical models include the drift-diffusion model and Bohm Quantum Potential (BQP) model for the carrier transport, the self-consistence Poisson-Schrodinger and k.p models for the MQW band structure, the spontaneous and piezoelectric polarization model for the built-in electric field. The carrier recombination process consists of Shockley-Read-Hall, Radiative, and Auger recombination terms. Taking Mg dopant ionization efficiency into account, the hole concentrations of HIL, EBL and p-GaN layer are all set to be $3e17 \text{ cm}^{-3}$. The radiative recombination coefficient (B) is kept constant at $5 \times 10^{-11} \text{ cm}^3 \text{ s}^{-1}$. To simplify the simulation, the

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light extraction efficiency is assumed to be 0.75. Other material parameters and the models for V-shaped pits used in the simulation can be found in reference [7].

III. RESULT AND DISCUSSION

The simulated and measured EQE curves are both shown in Fig. 1. The simulated EQE curve is in good agreement with the experiment, confirming the validity of the numerical model. In this simulation, the device is designed as a cylinder of 0.36 μ m in diameter. The V-shaped pit intersecting with the last QW is about 81nm in radius. Therefore, the density of V-shaped pits is about 1×10^9 cm⁻², and the V-shaped pits account for 20.3% area of the last QW.

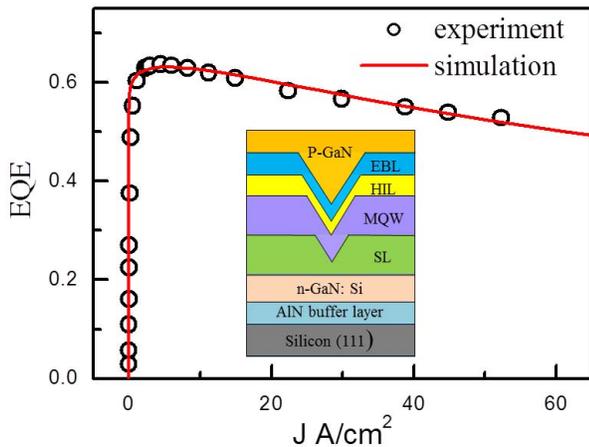


Figure 1. Experimental and simulated EQE curves of the reference LED. The inset shows the device structure with V-shaped pit.

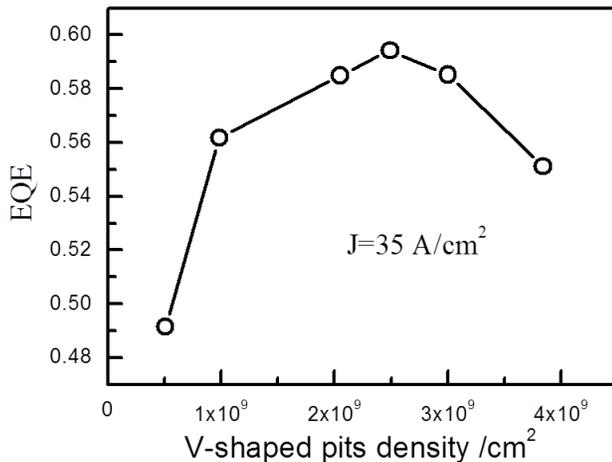


Figure 2. The dependence of the calculated EQE on the density of pits at 35A/cm²

To estimate the effect of the V-shaped pits density on the EQE of LED, a series of calculations for different density of pits with fixed size are performed. The dependence of the calculated EQE on the density of pits at 35A/cm² is presented in Fig. 2.

It is shown in fig.2 that the EQE is firstly enhanced and then reduced with an increase in the density of pits. The density corresponding to the maximum EQE value is about 2.5e9 cm⁻². There are two factors to cause this result. Firstly, the larger the density of pits is, the better it is for the injection of holes. Then, however, the excessive increase of the density could lead to the smaller area of emissive region, consequently resulting in poor optical output of LEDs.

IV. CONCLUSION

The simulated EQE curve of blue InGaN/GaN MQW LED with V-shaped pits is in good agreement with the experiment, confirming the validity of the numerical model. Then, LEDs with different density of pits are numerically investigated. The EQE is firstly enhanced and then reduced with an increase in the density of pits. Simulation results show that the optimal value of the density is about 2.5e9 cm⁻².

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