Numerical Simulation on Thermal-Electrical Characteristics and Electrode Patterns of GaN LEDs with Graphene/NiO_x Hybrid Electrode *

Quan-Xi Yan(闫泉喜)[1], Shu-Fang Zhang(张淑芳)[2**], Xing-Ming Long(龙兴明)[1,3], Hai-Jun Luo(罗海军)[1,3**], Fang Wu(吴芳)[1], Liang Fang(方亮)[1,4**], Da-Peng Wei(魏大鹏)[4], Mei-Yong Liao(廖梅勇)[1]

[1]*State Key Laboratory of Mechanical Transmission, College of Physics, Chongqing University, Chongqing 40044*
[2]*College of Software, Chongqing College of Electronic Engineering, Chongqing 401331*
[3]*College of Physics and Electronic Engineering, Chongqing Normal University, Chongqing 400047*
[4]*Chongqing Engineering Research Center of Graphene Film Manufacturing, Chongqing 401331*

(Received 14 January 2016)

The thermal-electrical characteristic of a GaN light-emitting diode (LED) with the hybrid transparent conductive layers (TCLs) of graphene (Gr) and NiO_x is investigated by a finite element method. It is indicated that the LED with the compound TCL of 3-layer Gr and 1 nm NiO_x has the best thermal-electrical performance from the view point of the maximum temperature and the current density deviation of multiple quantum wells, and the maximum temperature occurs near the n-electrode rather than p-electrode. Furthermore, to depress the current crowding on the LED, the electrode pattern parameters including p- and n-electrode length, p-electrode buried depth and the distance of n-electrode to active area are optimized. It is found that either increasing p- or n-electrode length and buried depth or decreasing the distance of n-electrode from the active area will decrease the temperature of the LED, while the increase of the n-electrode length has more prominent effect. Typically, when the n-electrode length increases to 0.8 times of the chip size, the temperature of the GaN LED with the 1 nm NiO_x/3-layer-Gr hybrid TCLs could drop about 7 K and the current density uniformity could increase by 23.8%, compared to 0.4 times of the chip size. This new finding will be beneficial for improvement of the thermal-electrical performance of LEDs with various conductive TCLs such as NiO_x/Gr or ITO/Gr as current spreading layers.

PACS: 85.30.−z, 66.70.Df, 72.20.−i DOI: 10.1088/0256-307X/33/7/078501

Nowadays GaN-based light-emitting diodes (LEDs) are widely used,[1,2] and it should be noticed that there are still some problems to be solved,[3] for example, the inhomogeneous current distribution and high junction temperature will seriously degrade performance and lifetimes of LEDs. [3,4] Generally, indium tin oxide (ITO) is applied as transparent conductive layers (TCLs) to spread current. ITO's high cost calls for research and development of some new alternative TCLs.[5] Owing to its high electrical conductivity and excellent transparency to visible light,[5−7] Gr has attracted considerable interests as a novel TCL to LEDs. However, the large work function mismatch of Gr (∼4.8 eV) and p-GaN (∼7.5 eV) will lead to a high operating voltage of Gr LEDs.[5−8] Inserting of ultrathin metal films between Gr and p-GaN and doping have been proposed to improve the Gr conductivity and work function.[5,6] On the other hand, metal films will decrease the transparency (e.g., merely 78% for 1 nm Ni/1 nm Au/monolayer Gr).[8] LEDs with multilayer Gr (>35) (MLG) were demonstrated to offer a record low forward voltage of ∼3.1 V, which is worthless due to very low transmission of MLG.[6] Zhang *et al.* revealed that insertion of an ultra-thin NiO_x layer can reduce the contact barrier between Gr and p-GaN, and the transparency is as high as ∼90% to the visible light,[7] so the NiO_x/Gr hybrid film can serve as a good electrode.[7,9,10] Introduction of a 3-nm-thick NiO_x was reported to enhance the overall Gr-LED performance by 1.5 times compared to the conventional ITO LEDs.[9] To date, no studies have provided the optimal combination of Gr layers and NiO_x thickness to obtain the best LED performance. Meanwhile, the electrode structure is proposed to be optimized to alleviate current crowding.[11] Increasing the number of p-electrodes and an appropriate arrangement of p- and n-electrode patterns were reported to facilitate current uniformity.[4,11] The influence of electrodes' pattern on the performance of LEDs with Gr/NiO_x hybrid electrodes is still unknown. The impact of Gr/NiO_x TCLs and electrodes' patterns on the thermal-electrical characteristics of LEDs should be investigated.

Therefore, in this Letter, the effects of TCLs combining Gr and a NiO_x layer and the electrode pattern parameters including p- and n-electrode lengths, p-electrode buried depth and the distance of n-electrode from the active area on the thermal-electrical characteristics of GaN LEDs are simulated, and the optical transmissions of different transparent electrical layers

*Supported by the Foundation of the State Key Laboratory of Mechanical Transmission of Chongqing University under Grant Nos SKLMT-KFKT-201419 and SKLM-ZZKT-2015Z16, the National High-Technology Research and Development Program of China under Grant No 2015AA034801, the National Natural Science Foundation of China under Grant Nos 11374359, 11304405, 11544010 and 11547305, the Chongqing Education Commission Scientific Project under Grant No KJ132209, the Natural Science Foundation of Chongqing under Grant Nos cstc2013jcyjA50031, cstc2015jcyjA50035 and cstc2015jcyjA1660, the Fundamental Research Funds for the Central Universities under Grant Nos CDJZR14135502, CDJZR14300050, 106112016CDJZR288805 and 106112015CDJXY300002, and the Sharing Fund of Large-scale Equipment of Chongqing University under Grant Nos 201512150017, 201512150029 and 201512150030.

**Corresponding authors. Email: lfang@cqu.edu.cn; roseymcn2000@foxmail.com; lhj19830330@126.com

© 2016 Chinese Physical Society and IOP Publishing Ltd

are calculated by the COMSOL software RF module. The obtained theoretical results will provide optimal fabrication parameters for high performance of GaN LEDs.

The steady-state method is used to simulate the Joule heating generated and transferred in GaN LEDs, the Joule heat Q of a current density $J_{\rm ex}$ with an electrical field E is

$$Q = J_{\rm ex} \times E, \tag{1}$$

where E is the gradient of electric potential ϕ, $E = \nabla\phi$ with ∇ being the gradient operator, determined by an external current density $J_{\rm ex}$ and electrical conductivity σ under static conditions,[13]

$$\nabla(\sigma \cdot \nabla\phi - J_{\rm ex}) = 0. \tag{2}$$

Each element in the active layer has an equivalent conductivity,

$$\sigma = \frac{l_{\rm e}}{V_j} J_{\rm e}, \tag{3}$$

where $l_{\rm e}$ is the elemental thickness of the mesh, V_j is the voltage drop between the active layers, and $J_{\rm e}$ is the elemental current density. Here $J_{\rm e}$ and V_j of each element satisfy the Shockley equation,[11,12] which describes the I–V characteristics of the LED,

$$J_{\rm e} = J_0[\exp(eV_j/nkT) - 1], \tag{4}$$

where J_0 is the saturation current density, n is the ideality factor, e is the elementary charge (1.6×10^{-19} C), k is the Boltzmann constant (1.38×10^{-23} J/K), and T is the absolute temperature. Here J_0 and n are dependent on the material quality and device structure. Nevertheless, J_0 is also affected by the temperature of the chip. The saturation current and n are set to be 4.72×10^{-22} A and 2.5, respectively.[13] In addition, the physical parameters of various materials are listed in Table 1 including electrical conductivity, thickness and thermal conductivity. The distribution of temperature field T at time t is

$$\rho c\frac{\partial T}{\partial t} = \nabla \cdot K_T \cdot \nabla T + Q, \tag{5}$$

$$k\nabla T = h(T_{\rm a} - T), \quad T_{\rm a} = T_{\rm bottom} = 300\,{\rm K}, \tag{6}$$

where Q is the heat source density; the temperature T at next time is determined by new temperature-dependent material parameters such as heat coefficient K_T; $T_{\rm a}$ and $T_{\rm bottom}$ are the ambient and sapphire bottom temperature settled at 300 K respectively, and h is the convection heat transfer coefficient equal to $20\,{\rm W/(m^2K)}$.[14] The current density uniformity is characterized by the standard deviation of the multi-quantum-well (MQW) x-axis surface current density, which is expressed by the number of mesh nodes n, the current density J_i of the ith mesh node and the average current density $\bar{J}$ read[14]

$$\sigma_j = \sqrt{\frac{1}{n-1} - \sum\nolimits_i^n (J_i - \bar{J})^2}, \ \bar{J} = \frac{1}{n}\sum\nolimits_i^n J_i. \tag{7}$$

Then transmissions of different TCLs are calculated by the Comsol in an rf frequency domain at 460 nm, and the refractive indexes of graphene and NiO_x are taken from the literature, $n = 2.0 + 1.1i$,[15] $n = 2.24 + 0.070i$,[16] respectively. The transmission of TCLs is equivalent to the ratio of the square of the electric field strength of two ports. The formulas are[16]

$$\nabla \times \mu_r^{-1}(\nabla \times E) - K_0^2\varepsilon_r E = 0, \quad \mu_r = 1,$$
$$\varepsilon_r = (n - ik)^2, \quad {\rm Tran} = \frac{{\rm Port}_2({\rm abs}(E^2))}{{\rm Port}_1({\rm abs}(E^2))}. \tag{8}$$

Then $T_{\max}$, the current density uniformity and the transmissivity of TCLs are applied as the optimal indices of the performance of the GaN LEDs, and the goal function is expressed as Eq. (9). To improve the GaN LED property significantly, we should reduce $T_{\max}$ and σ_j (current density uniformity is opposite), the cost should be as low as possible, cost $= \alpha \cdot K_{\rm G}[T_{\max}l - \min(T_{\max})] + (1-\alpha)\cdot k_j[\sigma_j m - \min(\sigma_j)] + [(1+\alpha)\cdot(1-{\rm Tran})]$,

$$K_{\rm G} = \frac{1}{T_{\max} - T_{\min}}, \quad k_j = \frac{1}{\sigma j_{\max} - \sigma j_{\min}}, \tag{9}$$

where $\alpha \in [0,1]$, l and m represent the data points in the simulation, $T_{max,l}$ and $\sigma_{j,m}$ are the data of lth and mth, Tran denotes the transmission of the corresponding TCLs.

Table 1. Physical parameters of various materials.[13]

Material	Sapphire	undoped GaN	n-GaN	MQWs	p-GaN	NiO_x	Graphene	p/n-pad
Thickness (μm)	80	2	2	0.075	0.1	0.001	0.00035	0.2
K (W/m·K)	38	130	130	130	130	8.2	5000	385
σ (S/m)			1×10^4	1×10^3	35	4.5×10^4	3.2×10^7	4.5×10^7

The three-dimensional finite element geometry involving TCLs of the proposed structure from the modeled GaN-LED chip size is 175 μm × 225 μm[7] in Fig. 1, and the model is simulated by using a computer.

The precision and accuracy of the simulation model are validated by using the operating voltages of LEDs with five different TCLs (280 nm ITO, single/multi-layer graphene (SLG/MLG), doped graphene, and graphene/NiO_x). In the numerical computation, the contact resistances of all kinds of electrodes are taken into account, the contact resistance is further characterized by using a circular transmission line model (CTLM).[7] The contact resistance between the NiO_x/graphene and p-GaN is $5.9\times10^{-4}\,\Omega\cdot{\rm cm}^2$, which is about 2–3 orders lower

than that of the graphene/p-GaN structure ($4.2 \times 10^{-2}\,\Omega{\cdot}\mathrm{cm}^2$), and also much lower than that of ITO/p-GaN or doped-graphene structure ($\sim 10^{-3}\,\Omega{\cdot}\mathrm{cm}^2$).[7,8] As shown in Fig. 2, the calculated operation voltages of the LED with the five different kinds of TCLs are compared with the experimental results from the literature[5–9] at an injection current of 20 mA. It is revealed that the relative errors between the calculated and the experimental data are in the range of 2.1%–6.5% (the error bars are presented in Fig. 2), indicating that our numerical method has high reliability.

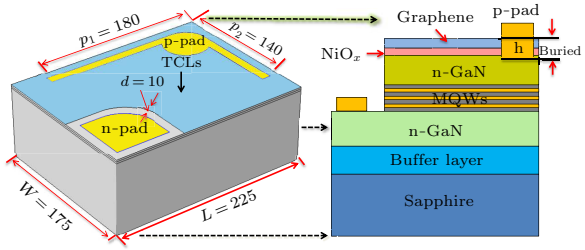

Fig. 1. The 2D/3D-dimensional structure of the GaN LED chip with the transparent electrical layers involved Gr and NiO_x (in units of μm).

The effects of different TCLs on the operation voltage of the LEDs are shown in Fig. 2. It demonstrates that the LED with 280 nm ITO TCL has the lowest operation voltage (~3.1 V). Chandramohan *et al.* reported that the operation voltage of the MLG LED is 3.21 V, which is owing to formation of ohmic contact at the MLG/p-GaN interface without the use of interlayer,[6] while the poor transmission of MLG (about 15%) is a fatal weakness of the MLG LED. SLG has a good transmission, while its small work function causes the largest operation voltage (6.15 V) for the SLG LED. However, the voltage of the LED with the SLG/NiO_x hybrid electrode is dramatically reduced from 6.15 V to 3.56 V, which is due to the fact that the ohmic contact property between graphene and p-GaN has been greatly improved by inserting the NiO_x buffer layer.[7] Meanwhile, the conductivity of graphene is reported to change non-linearly with layers number. When the layer number of graphene is more than 12, its resistivity is found to increase to $9 \times 10^{-6}\,\Omega{\cdot}\mathrm{m}$ which is almost close to the resistivity of the graphite.[16] Thus it is worth studying the dependence of the LED performance on the combination of graphene with different layers and the NiO_x with different thicknesses.

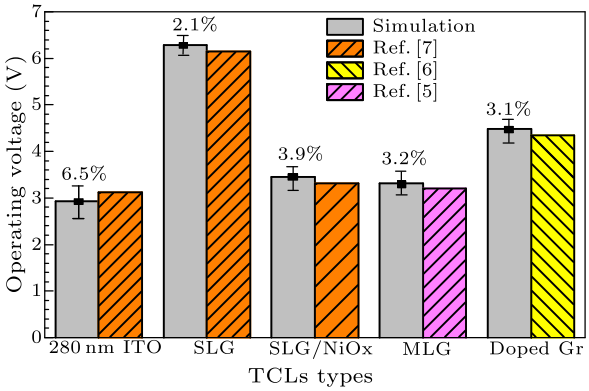

Fig. 2. The precision and accuracy of the operating voltage between the simulation results obtained from the model built and those from the literature[5–7] in which TCLs are ITO, Gr, Gr/NiO_x, doped Gr and MLG, respectively.

The effects of hybrid electrodes with the different combinations of 1–5 layers of graphene and 0–5-nm-thick NiO_x on the maximum temperature of the LED chip and the transmission of the TCLs are calculated, and the results are listed in Table 2. It shows that when only graphene (no NiO_x) is used, $T_{\max}$ of the chip decreases first and then increases with the number of Gr layers. This result can be explained as follows: (1) with the increase of the graphene layers, the current density decreases in the horizontal direction, thus $T_{\max}$ decreases firstly. (2) It is reported that with the increase of graphene layers, the conductivity of graphene decreases,[5] which causes both the transverse resistance and the joule heat of chip increase, thus $T_{\max}$ increases with the number of graphene layers. (3) The conductivity of graphene is found to change nonlinearly with the layer number,[16] thus in our simulation, the conductivity for the different graphene layers is not a constant, chosen according to the literature.[16] The lowest $T_{\max}$ of 324.7 K occurs at four Gr layers, which is consistent with the result of Xue *et al.*[14]

Table 2. The maximum temperature ($T_{\max}$) of the chip used for different combinations (NiO_x/Gr) at the injection current 20 mA, and transmission (Tran) of different hybrids (NiO_x/Gr).

Gr (layer)	1		2		3		4		5	
NiO_x (nm)	$T_{\max}$	Tran	$T_{\max}$	Tran	$T_{\max}$	Tran	$T_{\max}$	Tran	$T_{\max}$	Tran
0	327.05	97.72	326.12	95.51	325.10	93.37	324.74	91.29	325.78	89.28
1	322.86	95.19	321.17	93.47	319.61	90.52	318.17	88.46	321.77	87.37
2	322.00	92.93	321.07	92.11	319.01	88.46	318.07	87.07	321.66	85.03
3	321.85	91.05	320.74	90.55	318.94	87.01	317.96	85.72	321.56	83.59
4	321.45	89.77	320.56	88.28	318.86	86.25	317.85	84.28	321.46	81.27
5	321.04	88.28	320.08	87.01	318.66	85.11	317.72	83.06	321.34	80.05

When the NiO_x layer is inserted between graphene and p-GaN, it has been found that $T_{\max}$ of chip significantly becomes much lower than that without the NiO_x layer. With the increase of thickness of the NiO_x layer, $T_{\max}$ and transmission of TCLs reduce slowly, while $T_{\max}$ of the chip decreases first and then increases, and the transmission of TCLs decreases with the increase of the number of Gr layers. It is found that the LED with the TCL (three layers of Gr+(1 nm)NiO_x) hybrid electrode has the best per-

formance according to the goal function, σ_j and $T_{\max}$ are 4.825×10^6 A/m^2 and 319.6 K, which are 11% and 14.8% lower than those of four layers of the Gr LEDs, respectively. The transmission of TCL (three layers of Gr+1 nm NiO_x) is 90.52%, which is lower than that of the single-layer Gr, but higher than the experimental data (2 nm NiO_x+3-layer Gr) of 87%.[9] Therefore, we propose that 1 nm NiO_x+3-layer Gr as TCLs is the optimal electrode among the various combinations of NiO_x and Gr.

The distribution of temperature and MQWs' surface current density of the LEDs fabricated with 4-layer Gr (LED A) or 1 nm NiO_x/3-layer Gr (LED B) are shown in Fig. 3. The values of $T_{\max}$ of LEDs A and B are about 324.7 K and 319.6 K, respectively, and $T_{\max}$'s of two LED chips occur in regions near the n-electrode. This is attributed to the fact that the lateral current converges and crowds at the ground n-pad.

The current crowding in LED B has been relatively eased compared with LED A in the near n-electrode region. This is ascribed to the decreased contact resistance, which leads to more current passing from p-GaN to MQWs and n-GaN.[7] As a result, the vertical current increases in MQWs, thus correspondingly the light emission of GaN-based diodes with a NiO_x/graphene hybrid electrode was enhanced.[7–9]

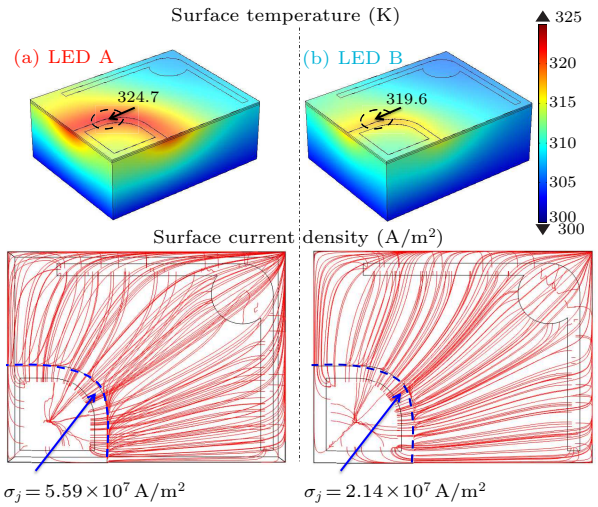

Fig. 3. The surface temperature and MQW surface current distribution of LED A with 4 layers graphene as TCLs (a) and of LED B with 1 nm NiO_x+3-layer graphene as TCLs (b).

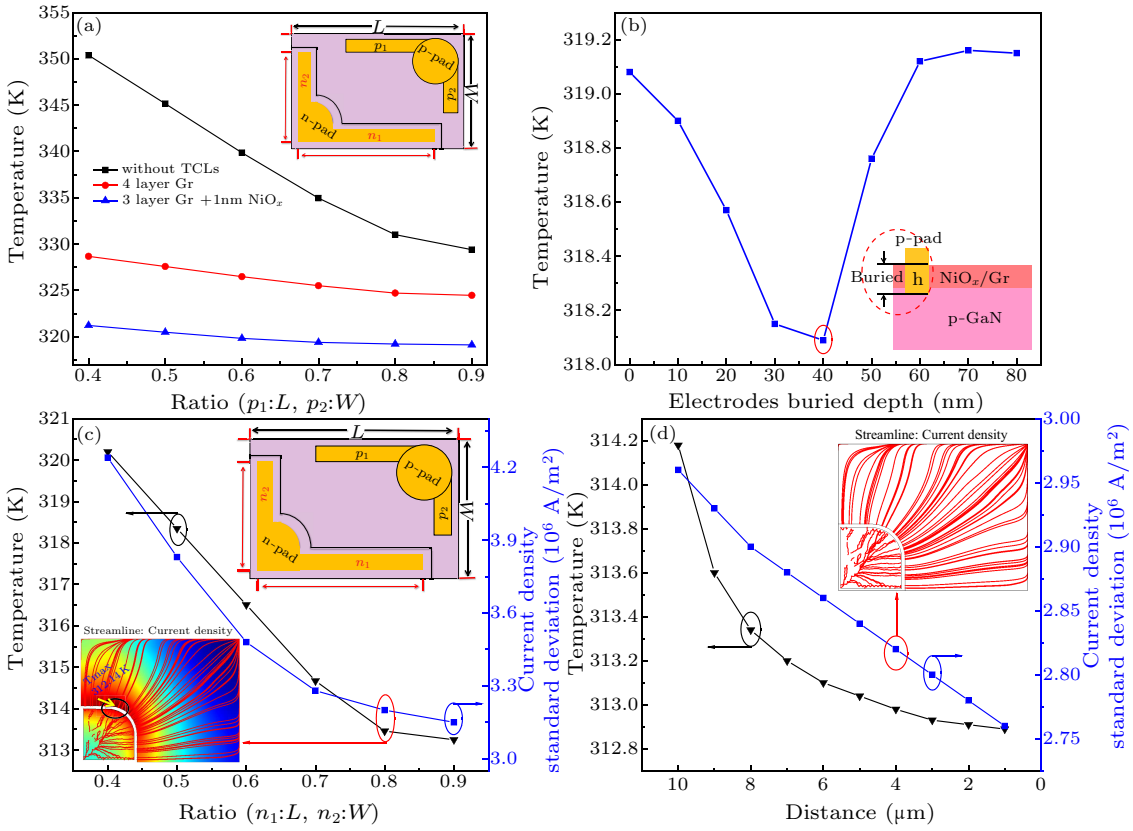

Fig. 4. (a) The maximum temperature with the ratio of the p-electrode length and the chip size. (b) The temperature with the electrode buried depth. (c) The maximum temperature and standard deviation of current density with the ratio of the n-electrode length and the chip size. (d) The maximum temperature and standard deviation of current density with the distance of the n-electrode from the active area.

To slow down the current crowding of LEDs, the effect of the electrode pattern on the thermal-electrical performance of LEDs based on a 3-layer Gr+1 nm NiO_x hybrid electrical layer is investigated. The electrode patterns include the p- and n-electrode lengths, p-electrode buried depth and the distance of the n-electrode from the active area. The obtained results are illustrated in Fig. 4.

As shown in Fig. 4(a), $T_{\max}$ of the chip decreases with the increase of the ratio of the p-electrode length to the chip size (p1: L, p2: W). When the ratio of p-electrode to chip size increases from 0.4 to 0.9, $T_{\max}$'s of the LEDs without TCLs, 4-layer Gr and 3-layer Gr+1 nm NiO_x decrease by 21℃, 4.22℃ and 2.10℃, respectively. This suggests that the increase of the p-electrode length on the chip could remarkably reduce $T_{\max}$ of the LEDs without TCLs while slightly decrease the ones with TCLs. At the same electrode patterns, the temperatures of the LEDs with TCLs are lower than the ones without TCLs, indicating that the TCLs play an important role in current spreading.

Youn *et al.* developed a novel Au/Cr/graphene electrode structure by adopting p-electrode metal (Cr) penetrating through the whole graphene to directly contact the p-GaN layer of the LED, and found that this new electrode structure can yield inter-plane (vertical) and in-plane currents (lateral) simultaneously, thus lowered the sheet resistance at the interface between the graphene and p-GaN, and improved the thermal stability in high-power GaN LEDs.[5] In our previous work,[14] we found that the electrode buried depth can significantly change the maximum temperature and the current density uniformity of 240-nm-ITO LEDs. Thus we are inspired to have a try to make p-electrode buried into the p-GaN in the Gr/NiO_x LEDs, and explore the relationship between current spreading performance and buried depth. The preparation process of the buried p-electrode is very similar to that of the conventional p- or n-electrode. For instance, Youn *et al.* reported that Gr films and GaN epilayers were etched by an inductively coupled plasma (ICP) etching process using O_2/N_2H_2 (graphene) and Cl_2/BCH_3 (GaN) source gases until the n-GaN layer was exposed for n-type ohmic contact.[8] The experimental details to fabricate the buried p- and n-electrodes can be referred to in the literature.[5]

Figure 4(b) shows the two-dimensional structure of the electrode buried and the dependence of $T_{\max}$ on the electrode buried depth h_{buried}. It reveals that $T_{\max}$ has a minimum value at the electrode buried depth of 40 nm, and $T_{\max}$ of the chip decreases 1 K in the LEDs with the NiO_x/Gr hybrid electrode structure. These results are similar to our previous findings in 240 nm ITO LEDs, i.e., the lowest $T_{\max}$ occurs at the electrode buried depth of 0.51 μm and $T_{\max}$ decreases about 2 K.[14]

When the p-electrode length is 0.8 times of chip sizes in the LEDs with 3-layer Gr+1 nm NiO_x as TCLs, the dependences of $T_{\max}$ and current density standard deviation on the n-electrode patterns are shown in Fig. 4(c). It is apparent that both $T_{\max}$ and current density standard deviation decrease markedly with the increase of the ratio of the n-electrode and the chip size (n1: L, n2: W). Typically, when the ratio is 0.8, $T_{\max}$ decreases about 7 K, the current density uniformity increases by 23.8%. In other words, an appropriate increase of the n-electrode length may play a key role in slowing the current crowding in the LEDs with TCLs. However, the chip luminous area will decrease with the increase of the n-electrode length, thus the n-electrode length cannot increase unboundedly, it needs to trade off with the luminance.

The dependences of $T_{\max}$ and the current standard deviation of the MQWs x-axis surface of TCLs on the distance of the n-electrode from the active area of the chip are shown in Fig. 4(d). It reveals that σ_j of MQW x-axis surface decreases dramatically while $T_{\max}$ reduces slowly with the decreases of the distance. The optimal distance is 4 μm (as shown by circles in Fig. 4(d), the current uniform distribution in the illustration) according to the goal function.

However, increasing the n-electrode length has greater effect than increasing p-electrode and buried depth or reducing the distance of the n-electrode from the active area. Due to the fact that the resistivity in the p-electrode metal (Cr/Au) is much smaller than that in the TCLs, the potential for the p-electrode layer can be regarded as an equal potential.[8] In comparison to the p-GaN layer, the resistivity of the TCLs is very small. Therefore, the current in the TCLs mainly radiates from the p-electrode horizontally to the n-electrode, the lateral current density of TCLs is much higher than the vertical current density passing from the p-GaN and MQWs to n-GaN.[11,12] The increase of the n-electrode length can reduce the current crowding density, equivalently the generated joule heat becomes less near n-electrode regions. Thus decreasing lateral resistance or increasing n-electrode length is essential to slow current crowding for the LEDs with high conductivity TCLs.

In summary, we have investigated the thermal-electrical performance of GaN-LEDs with different combinations of NiO_x/Gr as current spreading layers, and the electrode structures are also optimized. It is found that 1 nm NiO_x+3-layer Gr are the optimal combinations. Increasing the length of the n-electrode has most notable effect to decrease current crowding. Typically, when the n-electrode length increases to 0.8 times of the chip size, the temperature of the LEDs with the 1 nm NiO_x/3-layer-Gr hybrid TCLs could drop about 7 K and the current density uniformity increases by 23.8%.

References

[1] Wu L J et al 2012 *Chin. Phys.* B **21** 068506
[2] Kim J H et al 2000 *Appl. Phys. Lett.* **77** 1903
[3] Wang J H et al 2012 *Chin. Phys. Lett.* **29** 088502
[4] Wang P et al 2010 *Opt. Laser Technol.* **42** 737
[5] Youn D H et al 2013 *Nanotechnology* **24** 075202
[6] Chandramohan S et al 2014 *J. Appl. Phys.* **115** 054503
[7] Zhang Y et al 2012 *Nanoscale* **4** 5852
[8] Lee J M et al 2011 *Appl. Phys. Lett.* **99** 041115
[9] Wu C et al 2015 *Solid-State Electron.* **109** 47
[10] Chandramohan S et al 2013 *ACS Appl. Mater. Interfaces* **5** 958
[11] Sheu G J et al 2008 *J. Electrochem. Soc.* **155** H836
[12] Hwu F S et al 2010 *J. Electrochem. Soc.* **157** H31
[13] Long X M et al 2012 *Adv. OptoElectron.* **2012** 495981
[14] Xue S J et al 2014 *Chin. Phys. Lett.* **31** 028501
[15] Tyagi M et al 2013 *J. Mater. Res.* **28** 723
[16] Nirmalraj P N et al 2010 *Nano Lett.* **11** 16