3D Finite Element Strain Analysis of V-Shaped Pits in Light Emitting Diodes

Chung-Cheng Hsu[1], Chen-Kuo Wu[1], Chi-Kang Li[1], Tien-Chang Lu[2], and Yuh-Renn Wu[1]
[1]Graduate Institute of Photonics and Optoelectronics and Department of Electrical Engineering, National Taiwan University, Taipei 10617, Taiwan
[2]Department of Photonics and Institute of Electro-Optical Engineering, National Chiao-Tung University, Hsinchu 30050, Taiwan
E-mail:yrwu@ntu.edu.tw

Abstract—**In this paper, we have analyzed the strain distribution of the V-pits in light emitting diodes (LEDs). The special geometry and non-uniform distribution introduce the complicated strain and piezoelectric distribution, where it might affect the carrier injection. In the future, we will combine the calculated piezoelectric field with our in-house developed 3D drift-diffusion model to figure out how the carrier inject into LEDs with V-pits.**

Index Terms—**Elastic Strain; Quantum Wells (QWs); V-pit; Light Emmitting Diodes (LEDs); Threading Dislocations (TDs)**

Currently, LEDs are replacing the traditional illumination devices due to their higher energy efficiency. However, the notoriously high density of threading dislocations (TDs) existed in GaN LED has restricted the development of the LED. As we know, the TD might provide some nonradiative recombination center, or leakage path, which are disadvantages to the performance of the LED. However, some studies show that the V-pit, hexagonal pits with $(1\bar{1}01)$ side walls, existed in LEDs may influence the carrier injection path and might prevent the carriers from injecting into TDs. The electroluminescence (EL) measurements and transmission electron microscope (TEM)[1] data show that the V-pit region has a lower indium composition and thinner width than normal quantum well and barrier (QB). Although some researchers [2, 3] have proposed some numerical model to evaluate the influence the carrier injection in LEDs with V-pits, the models do not take into account for the complicated piezoelectric field distribution attributed to the complex strain distribution. In this paper, we have investigated the 3D strain distribution in detail and calculated the polarization field distribution. In the future, we will consider the calculated piezoelectric field and combine it with our 3D drift-diffusion model [4] to examine how the carrier inject into LEDs with V-pits.

Considering the linear response of the strain-stress relation, we can solve Hooke's law to calculate the strain in the system by 3D FEM method. The equations to be solved are as follows:

$$\frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{xy}}{\partial y} + \frac{\partial \sigma_{zx}}{\partial z} + f_x = 0 \quad (1)$$

$$\frac{\partial \sigma_{xy}}{\partial x} + \frac{\partial \sigma_{yy}}{\partial y} + \frac{\partial \sigma_{yz}}{\partial z} + f_y = 0 \quad (2)$$

$$\frac{\partial \sigma_{zx}}{\partial x} + \frac{\partial \sigma_{yz}}{\partial y} + \frac{\partial \sigma_{zz}}{\partial z} + f_z = 0 \quad (3)$$

$$\boldsymbol{\sigma} = [\sigma_{xx}, \sigma_{yy}, \sigma_{zz}, \sigma_{yz}, \sigma_{zx}, \sigma_{xy}]^T \quad (4)$$

$$\boldsymbol{\epsilon} = [\epsilon_{xx}, \epsilon_{yy}, \epsilon_{zz}, \epsilon_{yz}, \epsilon_{zx}, \epsilon_{xy}]^T \quad (5)$$

$$\boldsymbol{\sigma} = \boldsymbol{D\epsilon} \quad (6)$$

$$P^{pz} = \begin{pmatrix} e_{15}\epsilon_{xz} \\ e_{15}\epsilon_{yz} \\ e_{31}(\epsilon_{xx} + \epsilon_{yy}) + e_{33}\epsilon_{zz} \end{pmatrix} \quad (7)$$

where σ_{xx}, σ_{yy}, σ_{zz} are normal stresses, f_x, f_y, f_z are external distributed body force, and σ_{yz}, σ_{zx}, σ_{xy} are shear stresses. ϵ_{xx}, ϵ_{yy}, ϵ_{zz} are normal strains, ϵ_{yz}, ϵ_{zx}, ϵ_{xy} are shear strains, $\boldsymbol{D}$ is a 6×6 elastic tensor and composed with elastic constants c_{ij} (i, j = 1 $\sim$ 6). In the wurtzite structure, the nonzero terms are c_{11}, c_{12}, c_{13}, c_{33}, c_{44}, and c_{66}. Other coefficients are zero due to the hexagonal symmetric. P^{pz} is the strain-induced piezoelectric polarization, e_{15}, e_{31}, and e_{33} are piezoelectric coefficients.

Different samples have different diameters and indium compositions in the V-pit region, but they still have common characteristics. The width of the QW and QB in the V-pit region is around one-third of the QW and QB in the planar region and the EL emission peak has about 300$\sim$400 meV higher in the V-pit region. Consequently, we will follow these principles to design the simulation model of the LED with the V-pit. Fig. 1 shows the geometry and length parameters of our simulation model. The simulation structure consists of n/p-GaN layers, one $Al_{0.15}Ga_{0.85}N$ electron blocking layer (EBL) and six pairs of $In_{0.17}Ga_{0.83}N$/GaN MQWs. The diameter of hexagonal is 60 nm in the first QW and 174 nm in diameter in the EBL region. The thickness of QW/QB and EBL are 0.866, 4.33 and 8.66 nm in the V-pit region. The side of the calculation square is 440 nm which means the area ratio of the V-pit and total is around 10 % of the EBL region. The composition of QWs in the V-pit is 7 %.

Figure 2 shows the strain distribution in the cross sectional view along the V-pit center on the yz-plane. Since the lattice constant of InGaN is larger than GaN, the strain is compressed in the horizontal direction and tensile in the vertical direction and AlGaN has the different trend of the strain distribution due to the smaller lattice constant than GaN. However, the story is

978-1-4799-8379-7/151$31.00 ©2015 IEEE

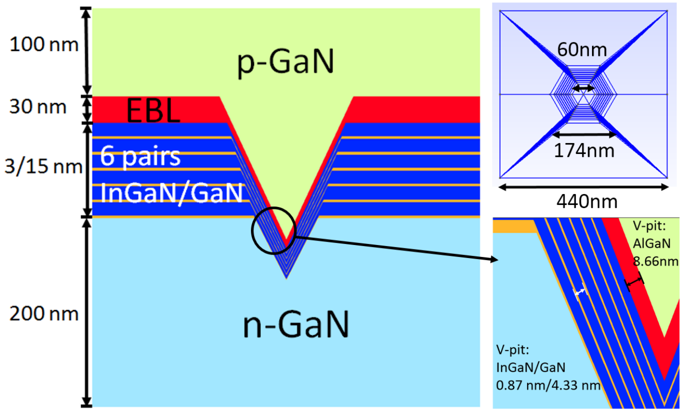

Fig. 1. Geometry of the simulation structure.

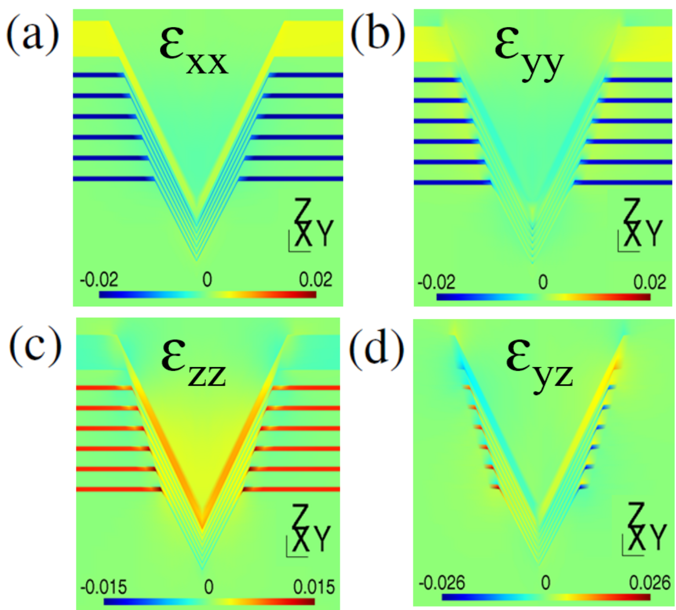

Fig. 2. Cross sectional view along the V-pit center of different strain (a) ϵ_{xx} on the yz-plane, (b) ϵ_{yy} on the yz-plane, (c) ϵ_{zz} on the yz-plane, and (d) ϵ_{yz} on the yz-plane.

different in the V-pit region. As shown in Fig. 2 (a) and (c), we can observe the strain in x and z direction is compressive in the V-pit region. It is because that the InGaN/GaN surface in the V-pit region are tilt that the compressive strain is partially in the x and z direction. Therefore, the ϵ_{zz} and ϵ_{xx} are compressive strain between InGaN/GaN and tensile strain between AlGaN/GaN surface. It is noted that the V-pit region is not infinite structure. The strain will be relaxed in the center of the V-pit and the corner of the planar/V-pits interfere the strain strength around the two ends of the V-pit will be smaller than the sidewall.

Fig. 2(b) shows the calculated strain ϵ_{yy} distribution in the cross sectional view along the V-pit center on the yz-plane. The ϵ_{yy} and ϵ_{xx} are both horizontal strain but different axis. However, due to the InGaN/GaN contact surface is much smaller along the y-axis and the ϵ_{xx} and ϵ_{zz} are compressive strain, the value of the ϵ_{yy} will be decided by two other strain components and is slight tensile in QW of the V-pit region.

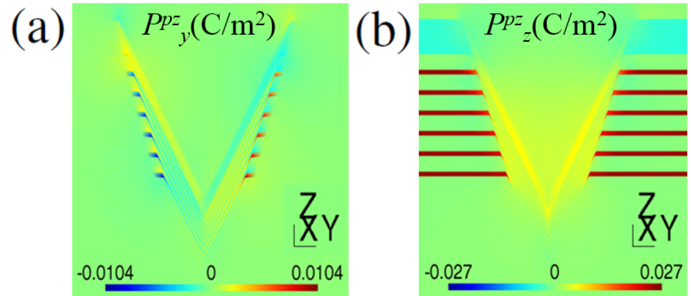

Fig. 3. Cross sectional view along the V-pit center of different piezoelectric polarization direction (a) piezoelectric polarization along y-axis on the yz-plane, and (b) piezoelectric polarization along z-axis on the yz-plane.

As we know, the ϵ_{xz} will be very small on the y-z and x-y plane, because there is less x-z and x-y component of the torque on the y-z plane. Hence, we won't show the ϵ_{xz} and ϵ_{xy} in this paper. Figs. 2(d) shows the calculated shear strain ϵ_{yz} distribution in the cross sectional view along the V-pit center on the yz-plane. There will be no torque in the conventional biaxial strain region, so the ϵ_{yz} in the planar region is close to zero. But the y-z torque induced by the strain force is not zero due to interface of the InGaN/GaN in the V-pit region has two components along the y-z direction. The y-z torque of different sidewalls has the same absolute value but with different sign on the corresponding plane because of the symmetric structure.

After getting the calculated strain, we use the Eqn. 7 to get the corresponding piezoelectric field distribution. In Figs. 3(a) and 3(b), the results shows P_z^{pz} is dominated in the planar region which is similar to the hypothesis of the infinite QW structure since there is no ϵ_{yz} appearing in the planar region. But, the P_y^{pz} indued by the ϵ_{yz} is large enough to be inevitable in the V-pit region.

In conclusion, we successfully simulate the strain distribution in the InGaN/GaN multiple QWs LED with V-pit. We find that the strain distribution of the V-pit region is much different from the conventional biaxial strain region due to the different InGaN/GaN and AlGaN/GaN surfaces.

In the future work, we will further investigate the electrical and optical property of the V-pit with 3D carrier transport model.

Acknowledgements

This work was supported the National Science Council of the Taiwan under Grant Nos. NSC-102-2221-E- 002-194-MY3 and MOST 104-2923-E-002-004-MY3.

References

[1] A. Hangleiter, F. Hitzel, C. Netzel, D. Fuhrmann, U. Rossow, G. Ade, and P. Hinze *Phys. Rev. Lett.* **95**, p. 127402, Sep 2005.
[2] Z. Quan, L. Wang, C. Zheng, J. Liu, and F. Jiang *Journal of Applied Physics* **116**(18), p. 183107, 2014.
[3] J. Kim, Y.-H. Cho, D.-S. Ko, X.-S. Li, J.-Y. Won, E. Lee, S.-H. Park, J.-Y. Kim, and S. Kim *Opt. Express* **22**, pp. A857–A866, May 2014.
[4] T.-J. Yang, R. Shivaraman, J. S. Speck, and Y.-R. Wu *Journal of Applied Physics* **116**(11), p. 113104, 2014.