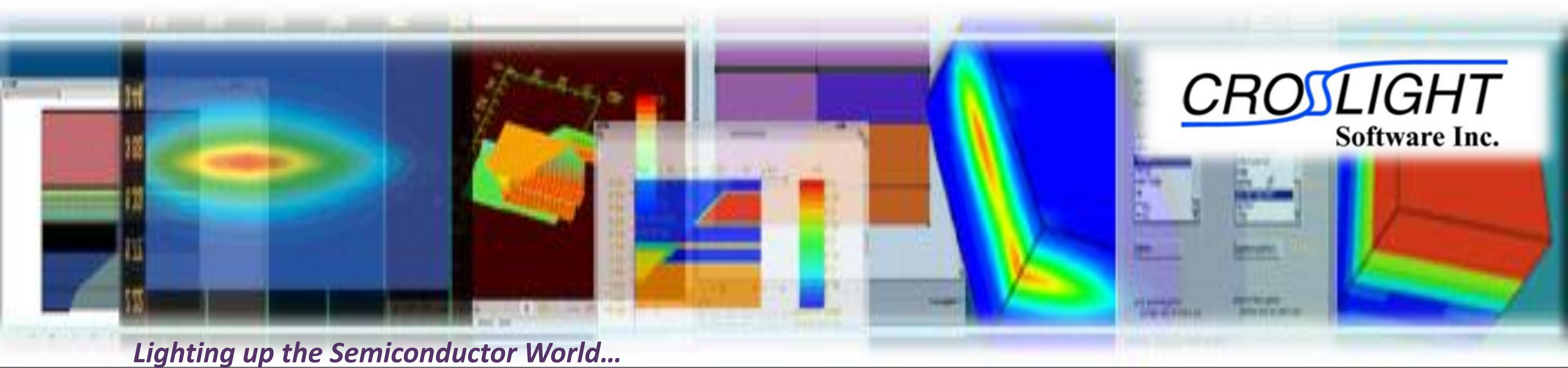
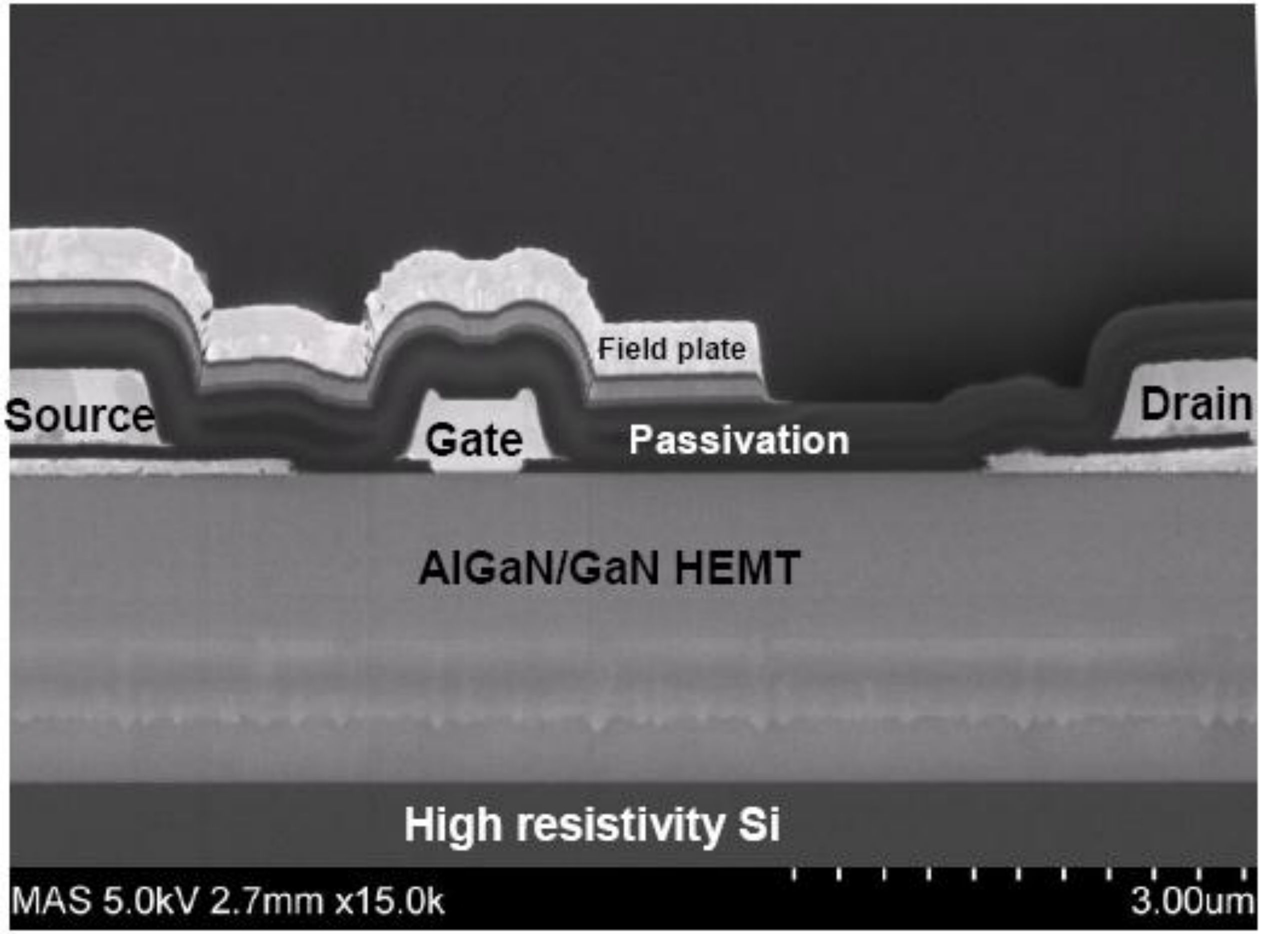


Simulation Study of Highly Stressed GaN Device on Silicon

Typical GaN HEMT on Silicon



Typical GaN LED on Silicon

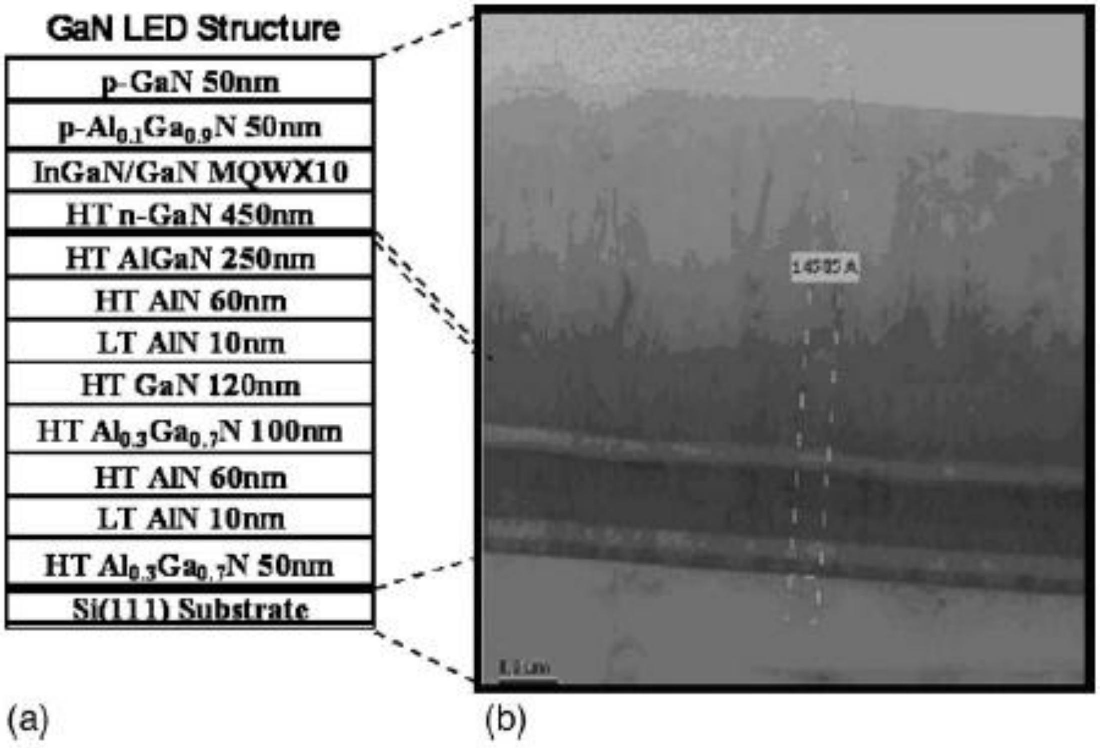


Figure 1. (a) Device structure and (b) cross-sectional TEM of InGaN LED prepared on Si(111) substrate.

Hsu, et.al.,Journal of The Electrochemical Society,
154 3 H191-H193 2007

Theoretical Models of Higly Stressed GaN MQW

MQW system assumed to be pseudomorphic with a single lattice spacing (size). Stress due to lattice mismatch in and around MQW layers are regarded as “internal stress”.

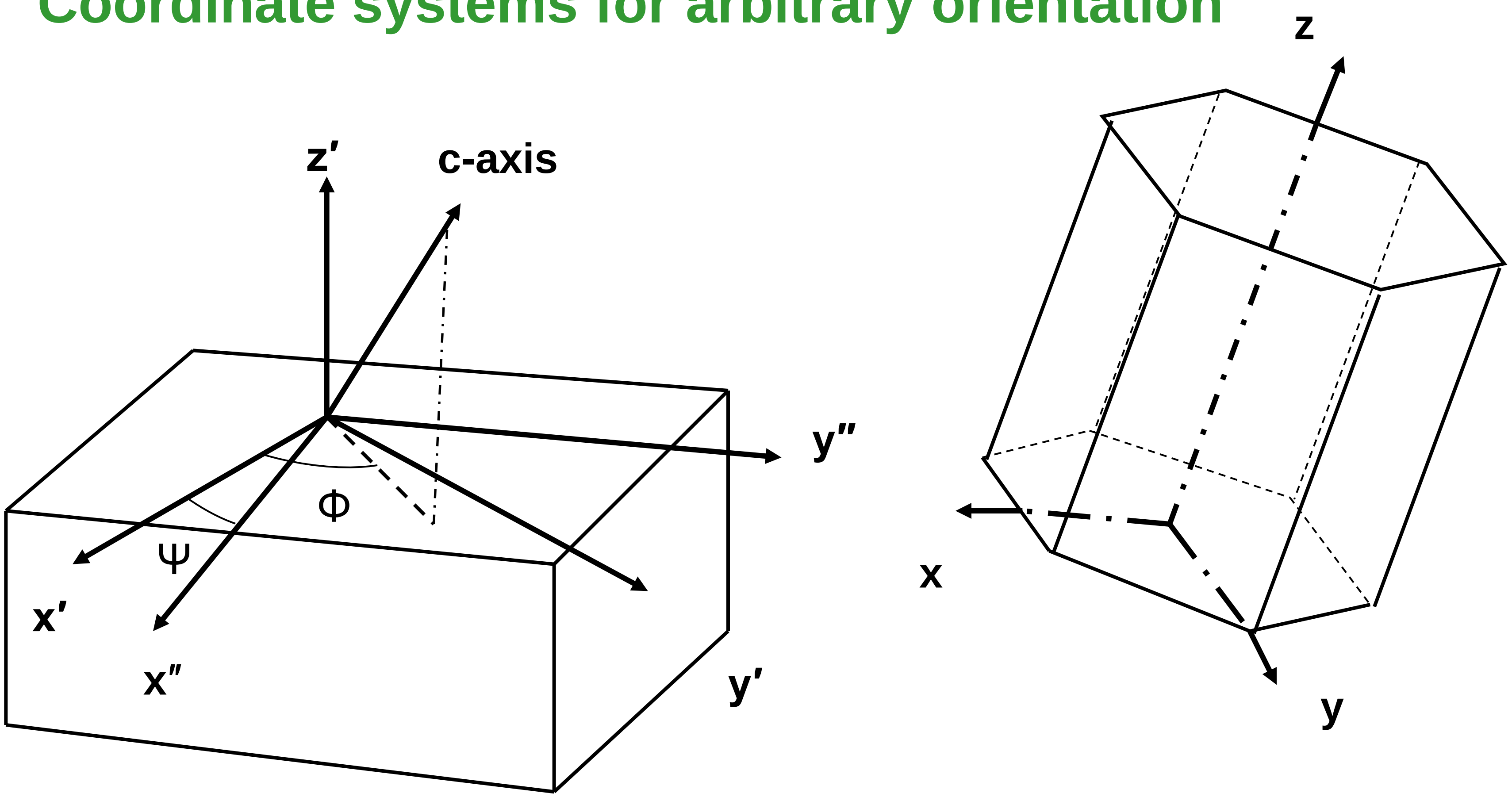
Large tensile stress due to lattice mismatch with silicon substrate are regarded as “external stress” .

External stress from silicon substrate alters device lattice spacing and thus modifies the strain terms in k.p band structure theory..

External stress significantly changes piezoelectric interface charge.

Large stress can cause change in many quantities such as bulk and MQW bandgaps, band offsets, quantum levels, lifetime and mobility.

Coordinate systems for arbitrary orientation



(x,y,z) – crystal coordinate where original Hamiltonian defined
(x',y',z') – growth coordinate system; z'=MQW normal
(x'',y'',z'') – waveguide system; z''//z'; y''=wave propagation direction

Hamiltonian

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$$H(\mathbf{k},\epsilon)=\begin{pmatrix} F & -K^* & -H^* & 0 & 0 & 0 \\ -K & G & H & 0 & 0 & \Delta \\ -H & H^* & \lambda & 0 & \Delta & 0 \\ 0 & 0 & 0 & F & -K & H \\ 0 & 0 & \Delta & -K^* & G & -H^* \\ 0 & \Delta & 0 & H^* & -H & \lambda \end{pmatrix} \begin{matrix} |U_1\rangle \\ |U_2\rangle \\ |U_3\rangle \\ |U_4\rangle \\ |U_5\rangle \\ |U_6\rangle, \end{matrix}$$

$$|U_1\rangle=-\frac{1}{\sqrt{2}}|(X+iY)\uparrow\rangle,$$

$$|U_2\rangle=\frac{1}{\sqrt{2}}|(X-iY)\uparrow\rangle,$$

$$|U_3\rangle=|Z\uparrow\rangle,$$

$$|U_4\rangle=\frac{1}{\sqrt{2}}|(X-iY)\downarrow\rangle,$$

$$|U_5\rangle=-\frac{1}{\sqrt{2}}|(X+iY)\downarrow\rangle,$$

$$|U_6\rangle=|Z\downarrow\rangle.$$

$$F=\Delta_1+\Delta_2+\lambda+\theta,$$

$$G=\Delta_1-\Delta_2+\lambda+\theta,$$

$$\lambda=\frac{\hbar^2}{2m_o}[A_1k_z{}^2+A_2(k_x{}^2+k_y{}^2)]+\lambda_\epsilon,$$

$$\theta=\frac{\hbar^2}{2m_o}[A_3k_z{}^2+A_4(k_x{}^2+k_y{}^2)]+\theta_\epsilon,$$

… etc

Strain dependence in k.p Hamiltonian

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Strain terms are in crystal (xyz) system and if MQW interface is not along z-axis, rotation matrices must be applied.

$$k'_i = U_{i\alpha} k_\alpha ,$$

$$\epsilon'_{ij} = U_{i\alpha} U_{j\beta} \epsilon_{\alpha\beta} ,$$

$$C'_{ijkl} = U_{i\alpha} U_{j\beta} U_{l\gamma} U_{j\delta} C_{\alpha\beta\gamma\delta} ,$$

$$K = \frac{\hbar^2}{2m_o} A_5 (k_x + i k_y)^2 + D_5 \epsilon_+ ,$$

$$H = \frac{\hbar^2}{2m_o} A_6 (k_x + i k_y) k_z + D_6 \epsilon_{z+} ,$$

$$\lambda_\epsilon = D_1 \epsilon_{zz} + D_2 (\epsilon_{xx} + \epsilon_{yy}) ,$$

$$\theta_\epsilon = D_3 \epsilon_{zz} + D_4 (\epsilon_{xx} + \epsilon_{yy}) ,$$

$$\epsilon_+ = \epsilon_{xx} - \epsilon_{yy} + 2 i \epsilon_{xy} ,$$

$$\epsilon_{z+} = \epsilon_{xz} + i \epsilon_{yz} ,$$

$$\Delta = \sqrt{2} \Delta_3 .$$

Pseudomorphic assumption

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$$\epsilon_{xx} = \epsilon_{xx}^{(0)} + \epsilon_{xz} \frac{\sin\theta}{\cos\theta},$$

where $\epsilon_{xx}^{(0)} = (a_s - a_e)/a_e$ and $\epsilon_{zz}^{(0)} = (c_s - c_e)/c_e$

$$\epsilon_{yy} = \epsilon_{xx}^{(0)},$$

$$\epsilon_{zz} = \epsilon_{xz} \frac{\cos\theta}{\sin\theta} + \epsilon_{zz}^{(0)},$$

$$\epsilon_{xy} = \epsilon_{yz} = 0,$$

* e labels any epilayer in MQW systm;
* s labels “substrate” which in this case is NOT the silicon substrate but the bulk layer of device with largest volume.
* Elastic energy is minimized to find the device lattice spacing vertical to MQW:

$$W = \tfrac{1}{2}[C_{11}\epsilon_{xx}^2 + C_{11}\epsilon_{yy}^2 + C_{33}\epsilon_{zz}^2 + 2C_{12}\epsilon_{xx}\epsilon_{yy} + 2C_{13} \times (\epsilon_{xx}\epsilon_{zz} + \epsilon_{yy}\epsilon_{zz}) + 4C_{44}\epsilon_{xz}^2].$$

Effect of stress due to silicon substrate

Silicon substrate causes large tensile stress (external stress in GPa) on MQW system which alters the device lattice spacing a_s and c_s according to stiffness matrix of bulk layers of the device.

$$\tau_{ij} = c_{ijkl}\epsilon_{kl}$$

where tau is external stress in GPa and epsilon is strain tensor. Stiffness matrix in short hand notation is given by

$$\begin{pmatrix} c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\ c_{12} & c_{11} & c_{13} & 0 & 0 & 0 \\ c_{13} & c_{13} & c_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{66} \end{pmatrix}$$

MQW lattice spacing change due to silicon

External stress tensor caused by silicon is given in GPa in (x' y' z') system. Rotation matrix is applied to convert to stress in (x y z) of original hexagonal lattice system. Then strain tensor in original system is computed according to

$$\tau_{ij} = c_{ijkl}\epsilon_{kl}$$

Finally device lattice spacing change due to external stress is approximated by

a_s(ext) = a_s [1 + (epsilon_xx+epsilon_yy)/2]
c_s(ext) = a_s (1 + epsilon_zz)

Given MQW system lattice spacing, strain tensor in k.p theory can be determined and band structure calculation can proceed as usual.

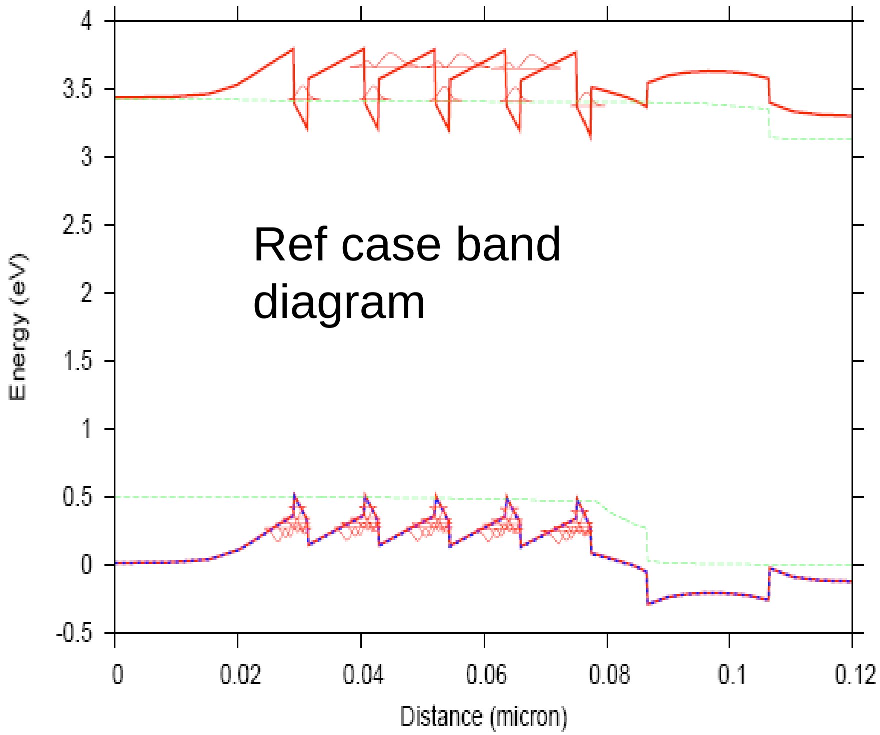
Simulation demo example: GaN LED on silicon

InGaN/GaN 5 wells 15 percent indium, 2.5 nm well thickness.

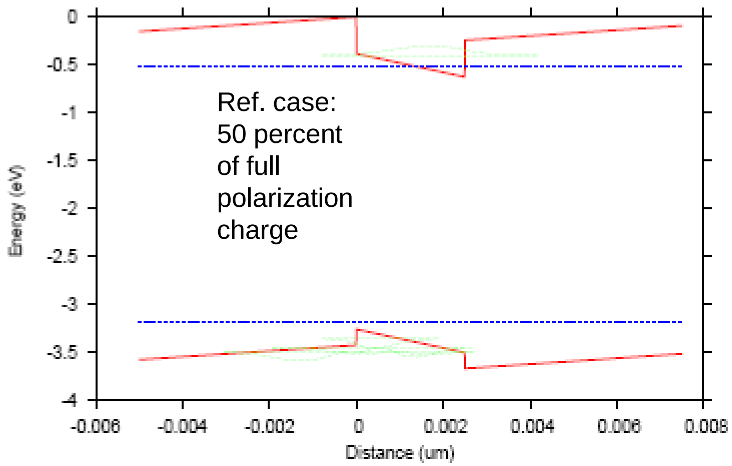
Main cause of IQE droop comes from polarization charge lowering of EBL which assumes to take band offset value of 0.5.

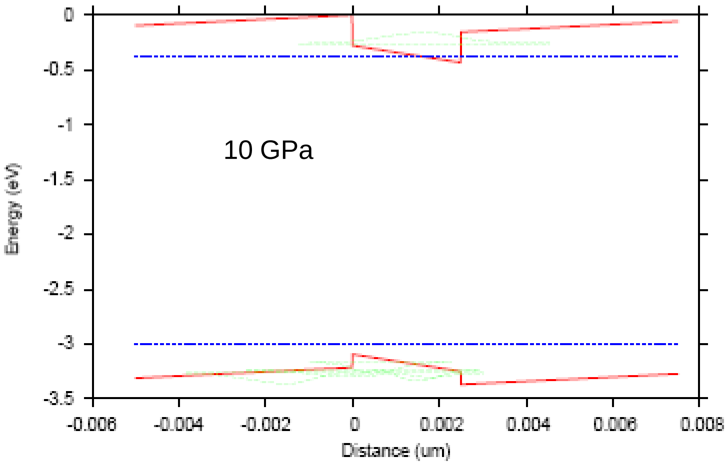
Effect of Auger recombination leakage is assumed to be negligible.

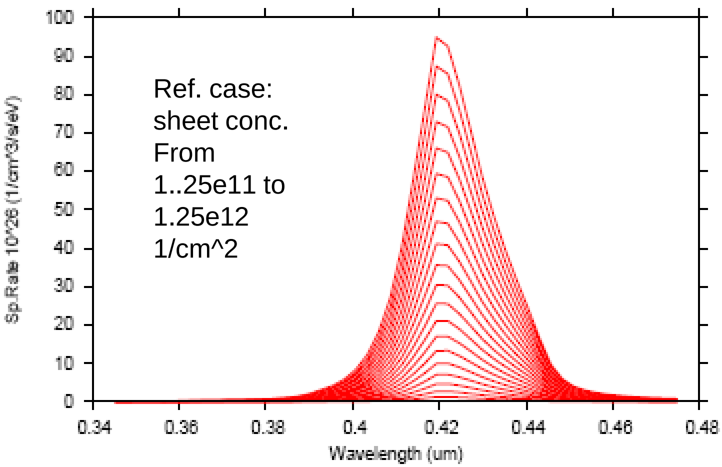
Only effects of external stress to polarization charge and k.p MQW structure are considered in this study.

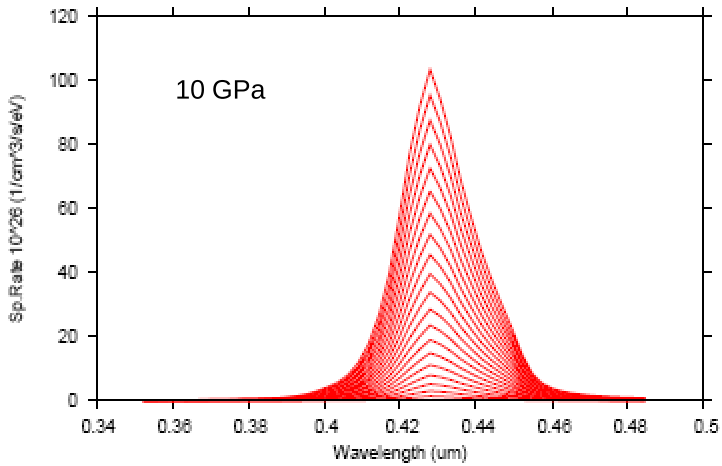


GaN LED on silicon stress_xx=stress_yy=10 GPa

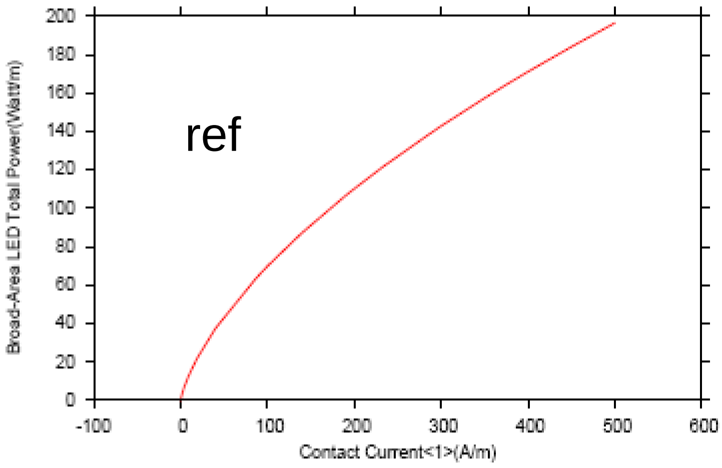


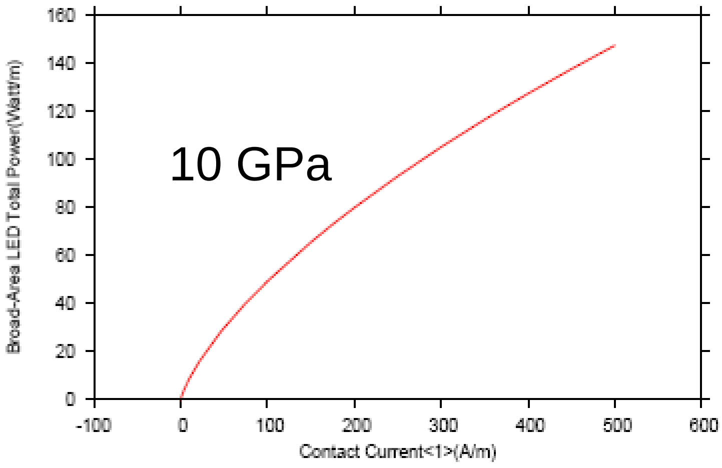


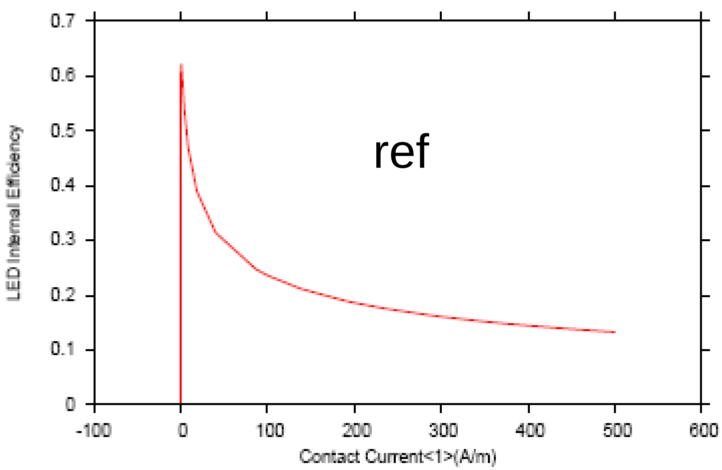


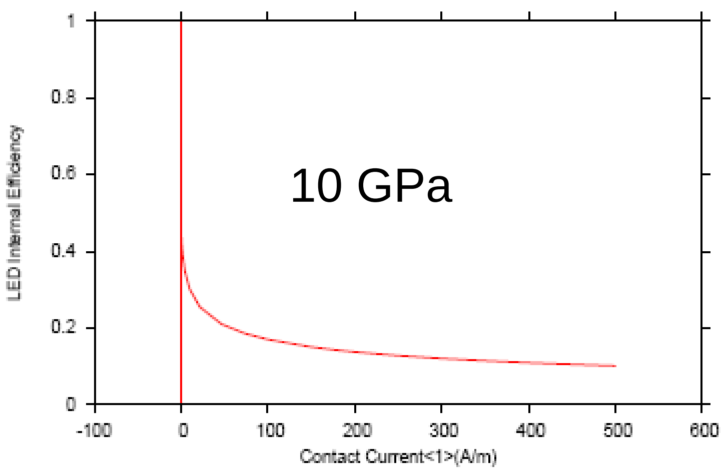


GaN LED on silicon stress_xx=stress_yy=10 GPa

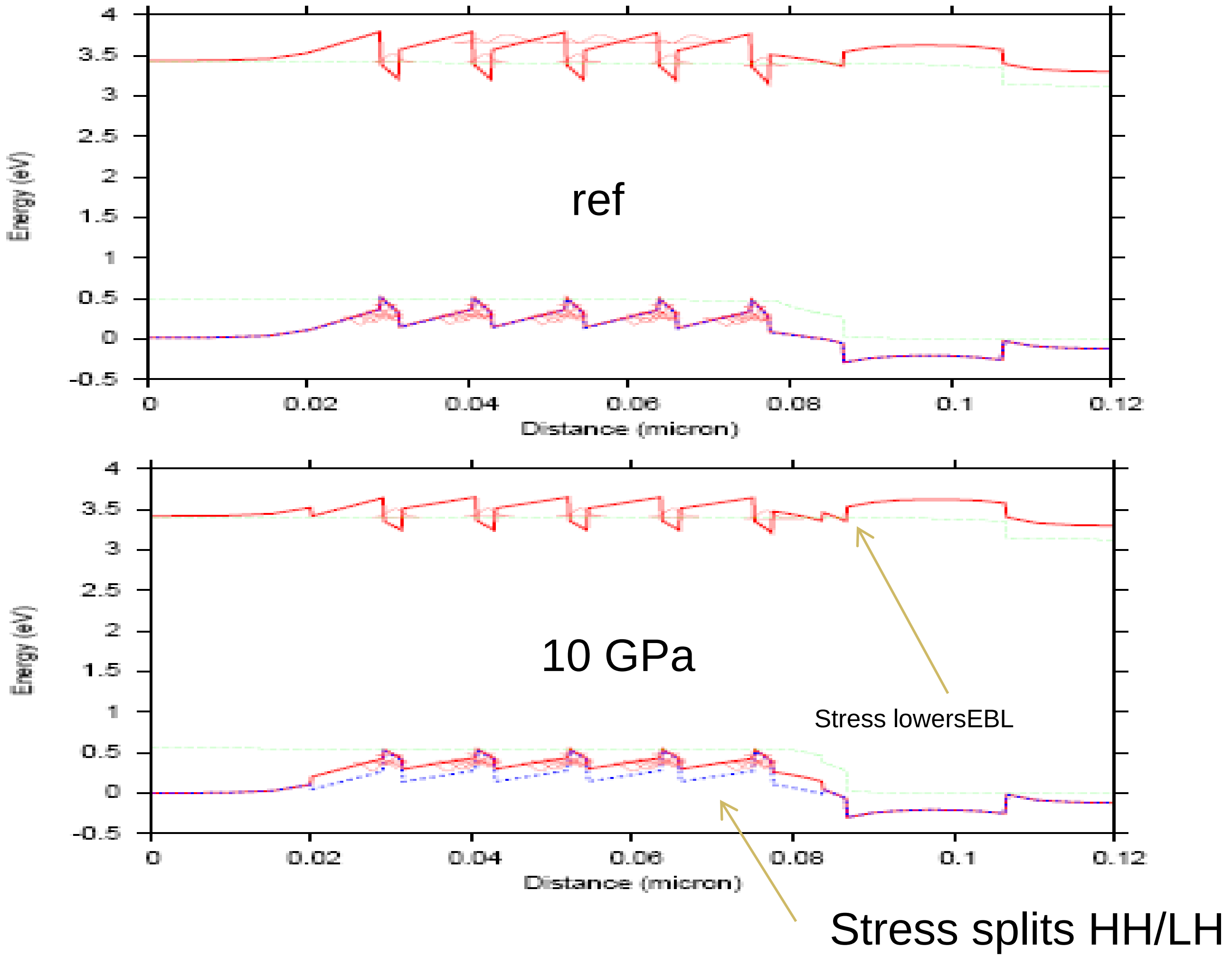








GaN LED on silicon stress_xx=stress_yy=10 GPa



Summary

Crosslight software ready to simulate GaN devices grown on silicon with arbitrary crystal orientations. Using InGaN/GaN LED/silicon as demo example in a k.p band structure theory including piezo-electric effects, we find

(1) Tensile stress from silicon substrate reduces the bandgap of MQW and results in longer emission wavelengths..

(2) Piezo-electric charges are reduced in QW while they are increased in other parts of the device, including the EBL interfaces.

(3) Degradation of IQE results from increased piezo-electric charges on EBL interfaces which furthers lowers the EBL potential and causes more overflow leakages.

A Glimpse

Crosslight Software

- A leading TCAD provider since 1993
- The world's No.1 TCAD simulator for optics and photonics application
- The world's first commercialized TCAD for Laser Diode
- Customer list extends to hundreds of companies, research institutions and universities world wide.
- Originally licensed from the National Research Council Canada and later from Stanford University
- Complete product portfolio for 2D/3D semiconductor device simulation
- *Café-time Simulator*. Windows based, user friendly graphic user interface makes simulation more enjoyable.

Creators of Award Winning Software

CROSSLIGHT
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