Effects of Crystal Orientation on the Optical Properties of GaN based Devices

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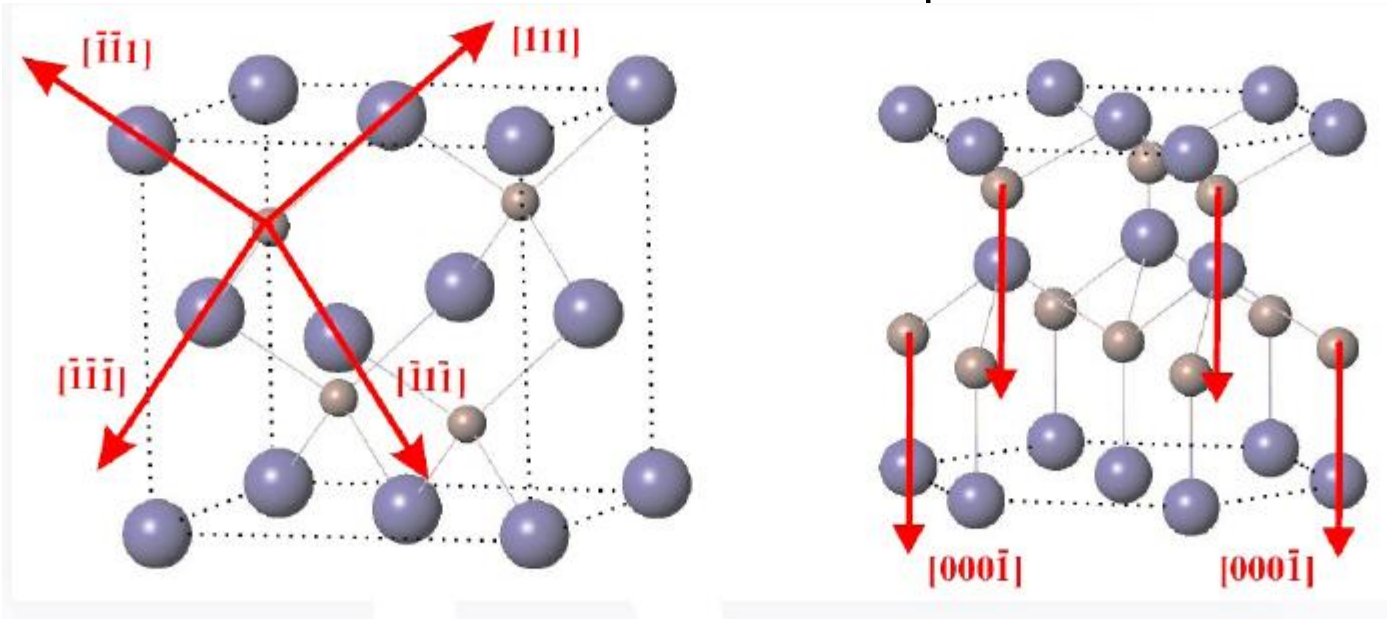
Outline

- Crystal orientation and polarization
- k.p method for QW of arbitrary orientation
- Results for InGaN/GaN QW
- LD performance

Spontaneous Polarization

Cubic
zero net polarization

Hexagoanl
Non-zero net
polarization



N. G. Thillosen (PhD thesis: Spin-Bahn-Wechselwirkung in niedrigdimensionalen AlxGa1−xN/GaN-Elektronengasen)

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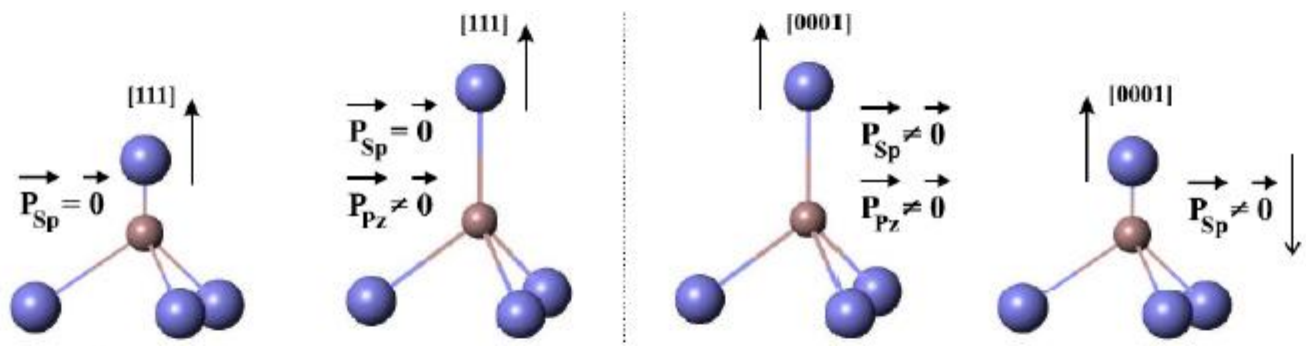
Piezoelectric polarization

Cubic

Hexagonal



No strain

Bi-axial strain

No strain

Bi-axial strain

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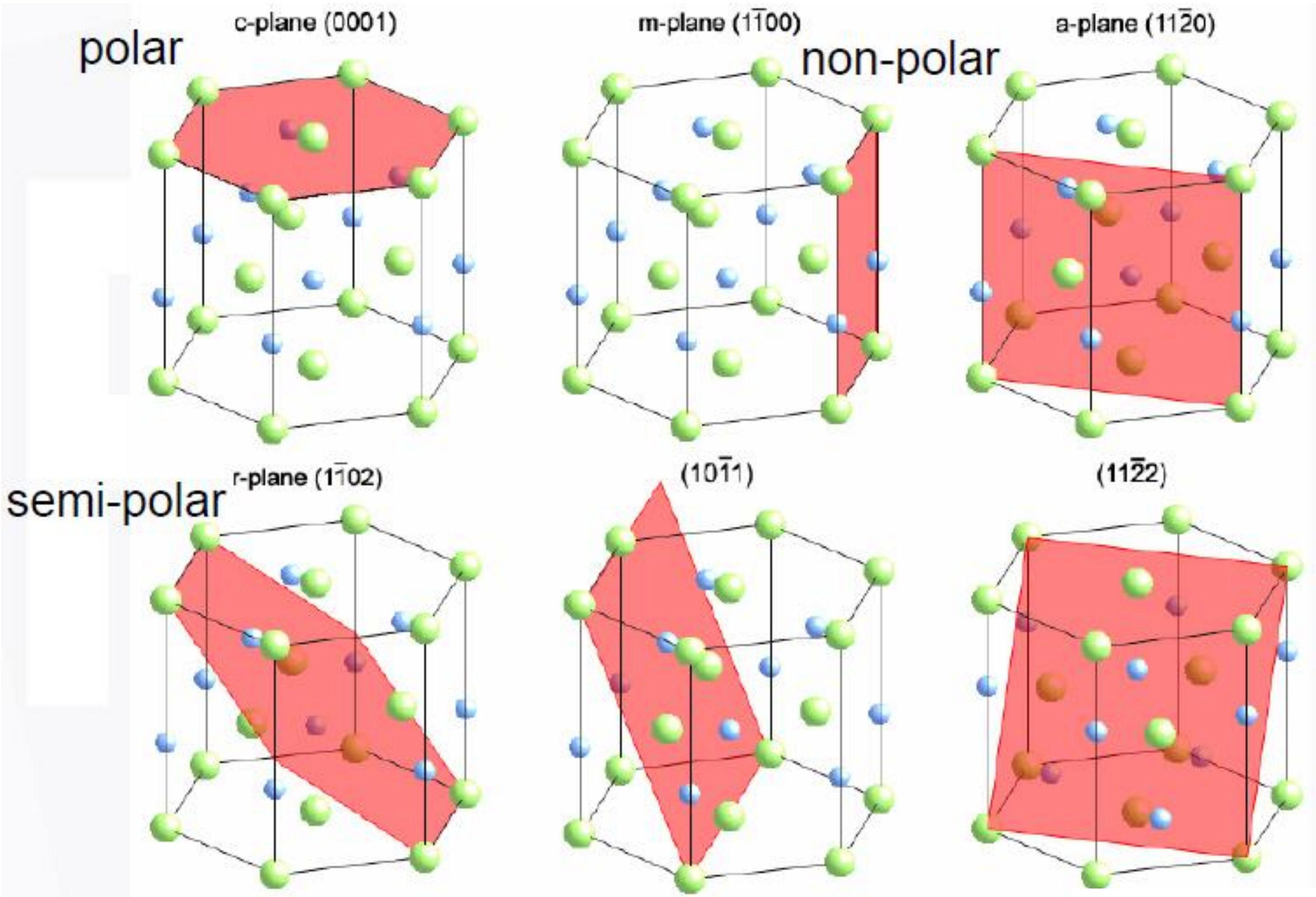
Alternative growth orientations



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Band structure

- Conduction band is treated by parabolic model

$$\Psi_n^{c\eta}(z,\vec{k}_t) = \frac{1}{\sqrt{V}} e^{i\vec{k}_t \cdot \vec{r}_t} \phi_n(z) \,|\, S\eta >$$

S is spherical wavefunction, η is spin, $\phi_n(z)$ is the envelope function of *n*th subband

Valence band

- Valence band is treated by 6x6 k.p method, including top three valence bands

$$H(\vec{k},\varepsilon) = H(\vec{k}) + D(\varepsilon)$$

strain

$$H(\vec{k},\varepsilon)|\Psi> = E(\vec{k})|\Psi>$$

For quantum well

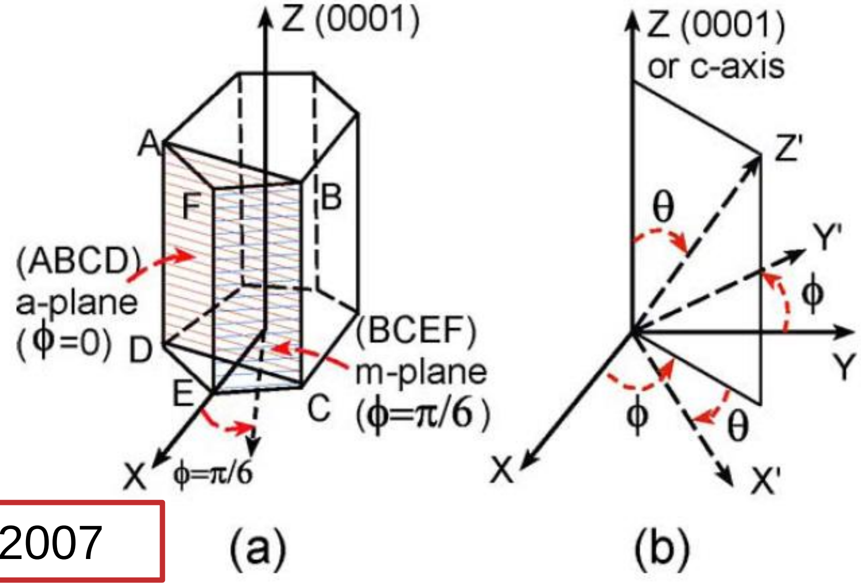
$$\Psi_m^v(z,\vec{k}_t) = \frac{1}{\sqrt{V}} e^{i\vec{k}_t\cdot\vec{r}_t} \sum_{i=1}^{6} g_m^i(z,\vec{k}_t) U^i$$

g_m is the envelope function of the *m*th subband
U^i are basis functions

Rotation

Hamiltonian for arbitrary rotation $H(k')$ can be obtained by rotation matrix

$$U = \begin{pmatrix} \cos\theta\cos\phi & \cos\theta\sin\phi & -\sin\theta \\ -\sin\phi & \cos\phi & 0 \\ \sin\theta\cos\phi & \sin\theta\sin\phi & \cos\theta \end{pmatrix}$$



JQE, v43,p1175,2007

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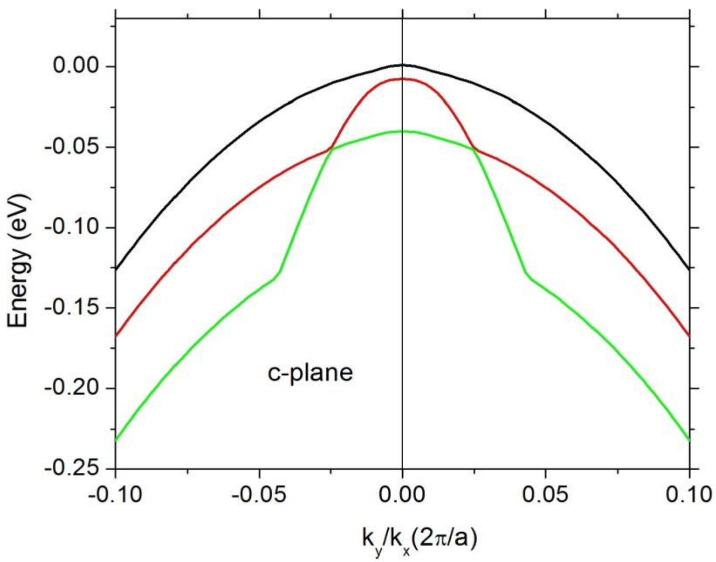
Strain tensor for arbitrary crystal orientation

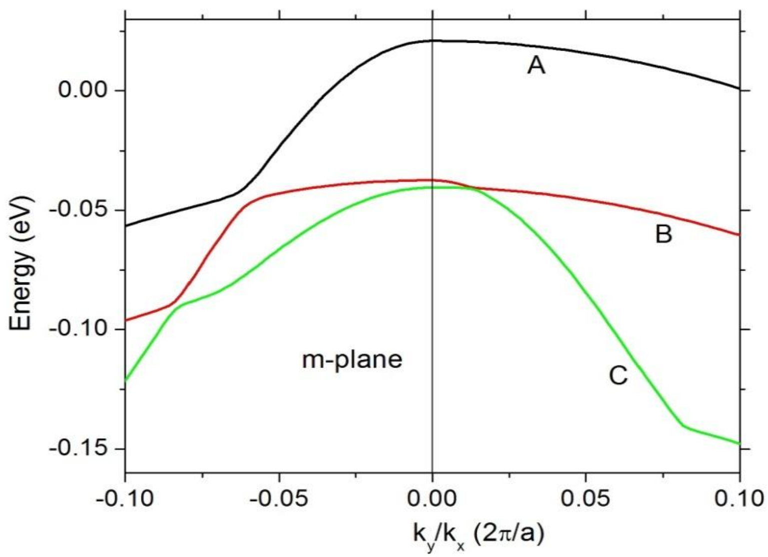
- Strain coefficients for arbitrary crystal orientation are calculated by minimizing the elastic energy under the conditions for pseudo-morphic growth.

$$W = \frac{1}{2}\sum_{i=1}^{6}\sum_{j=1}^{6}\int C_{ij}\varepsilon_i\varepsilon_j dV$$

PRB, v59, 4725, 1999

Anisotropic band structure





c-plane: isotropic

m-plane: anisotropic band structure. Smaller effective mass in y-direction

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Optical momentum matrix

Optical momentum matrix elements for transition between conduction band *n* and valence band *m* are defined as

$$|M_{nm}^{\eta}|^2 = |\hat{e} \cdot M^{\eta}|^2$$

$$= |< \Psi_n^{c\eta} | \hat{e} \cdot p | \Psi_m^{v} >|^2$$

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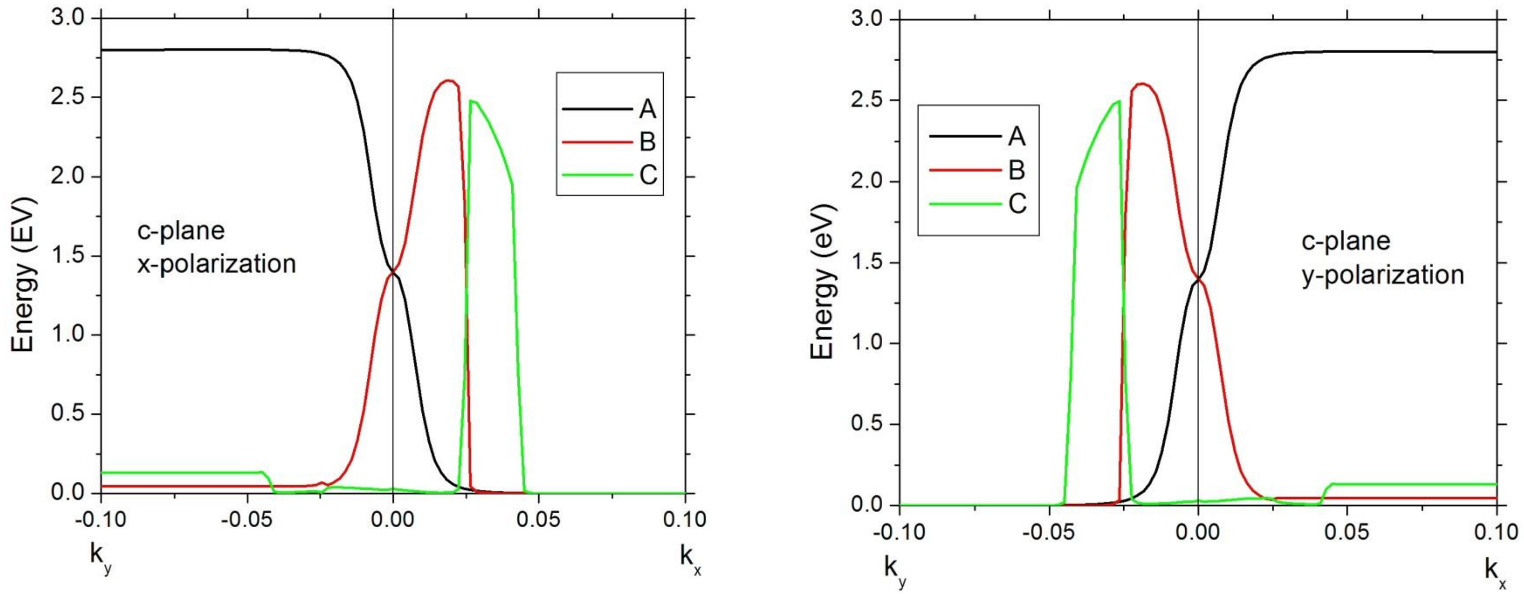
Optical matrix elements: c-plane



A,B,C are for transitions from conduction band to top three valence bands. Integrating over (kx-ky) plane, optical matrix elements are NOT dependent on E-field polarization on x-y plane.

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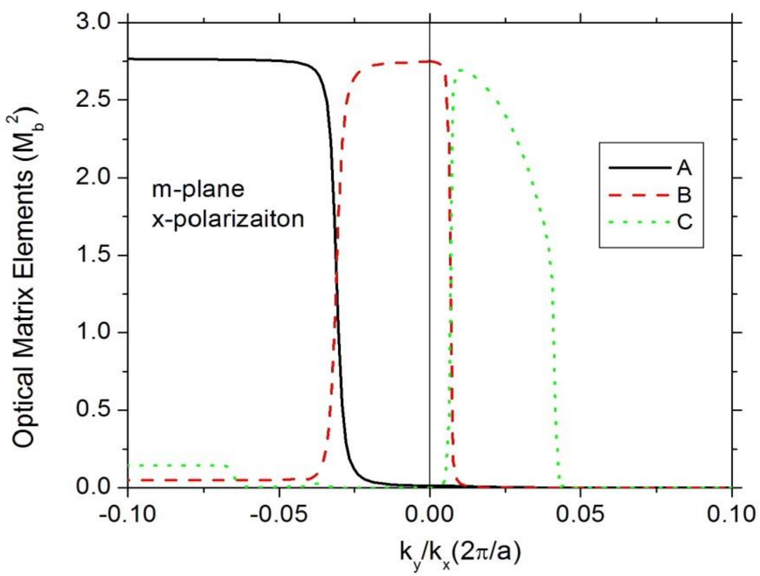
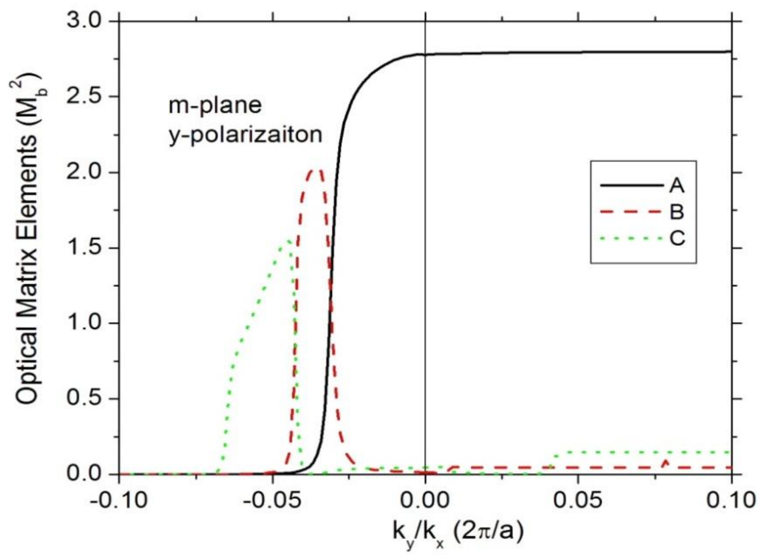
Optical matrix elements: m-plane





A,B,C are for transitions from conduction band to top three valence bands. Optical matrix elements are dependent on polarization.

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Optical gain

- Optical gain is calculated by

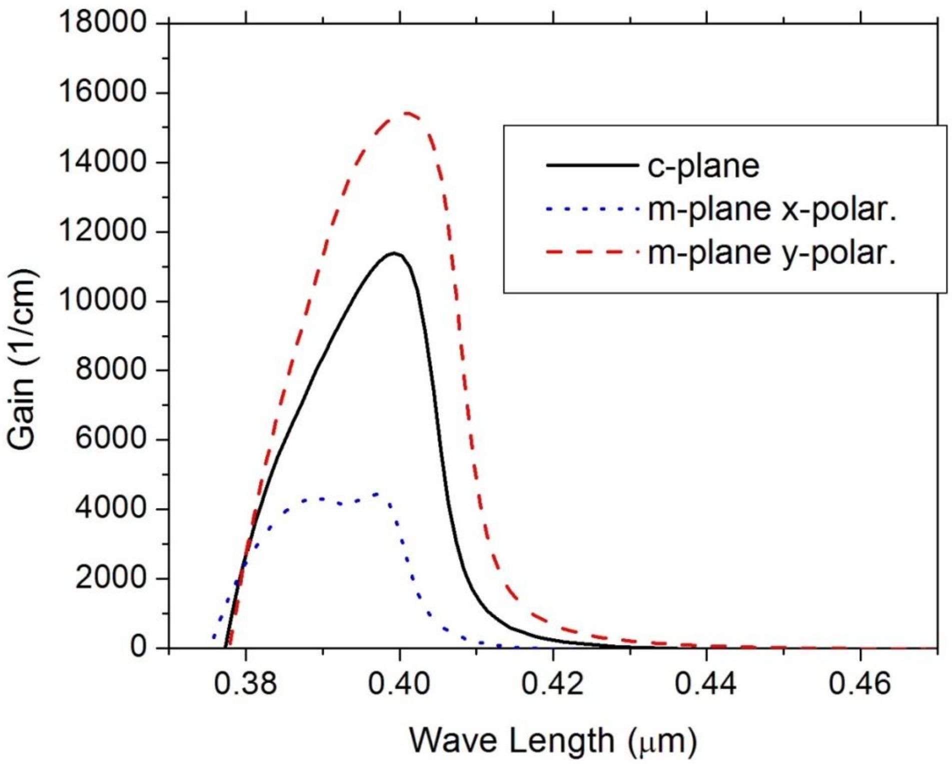
$$g(\omega)=\frac{q^2}{n_r c\varepsilon_0 m_0^2 \omega d_\omega}\sum_{n,m,\eta}\int d\vec{k}_t\,|M_{nm}^{\eta}|^2\,[f_n^c - f_m^v]L(\omega)$$

L(ω) is broadening function. Note 2D integration is necessary except for c-plane QWs, where the band structure is isotropic. Similar 2D integration for spontaneous rates as well.

Optical gain for different orientations

$30nm-In_{15}Ga_{85}N/GaN$ Quantum well at carrier density of $6.67e25/m^3$

No polarization charge in all cases



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Effects of crystal orientation: from c-plane to m-plane

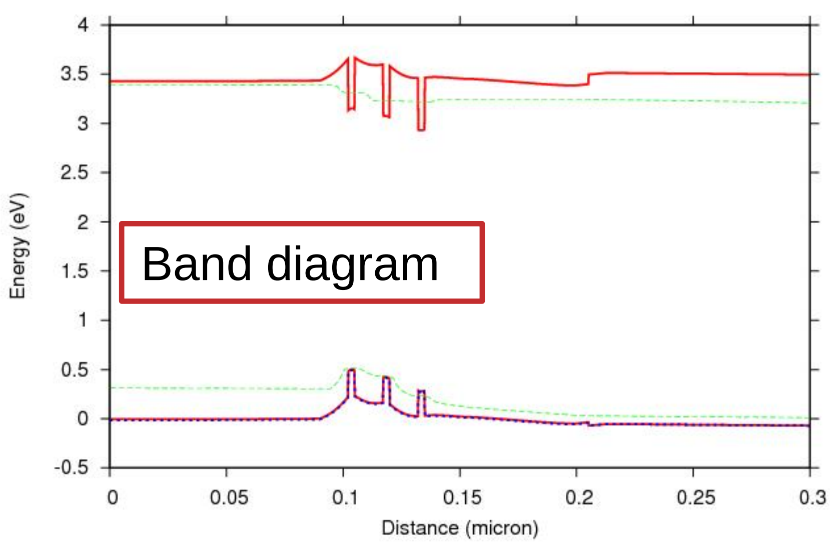
- No polarization charge
- Optical gain: polarization dependent, enhanced in y-polarization
- Transport: effective mass is reduced

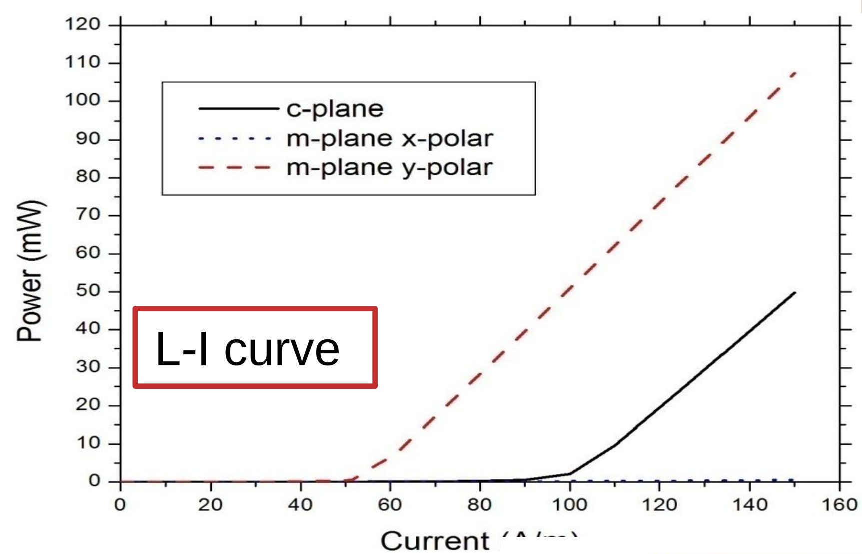
How do these affect the laser performance?

Laser performance: finite-element simulation

Edge-emitting laser active region:
30-nm $In_{15}Ga_{85}N/GaN$ QW (x3)

No polarization charges in all cases





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