

# Valence band engineering of AlN, InN and AlInN

---

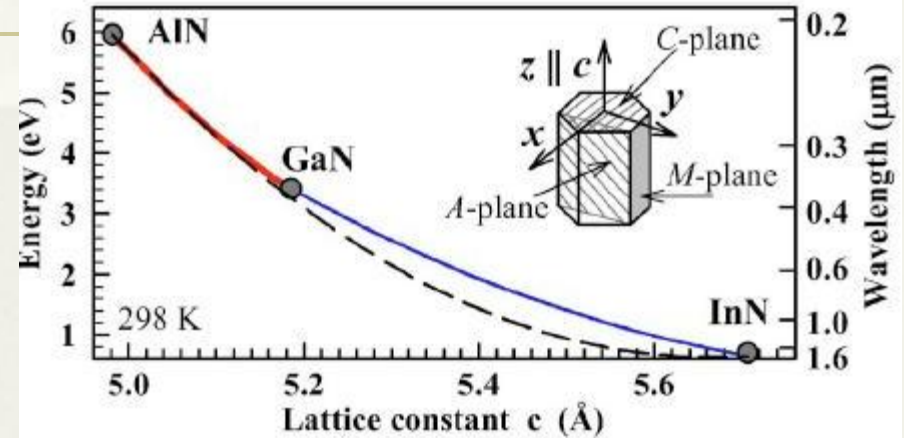
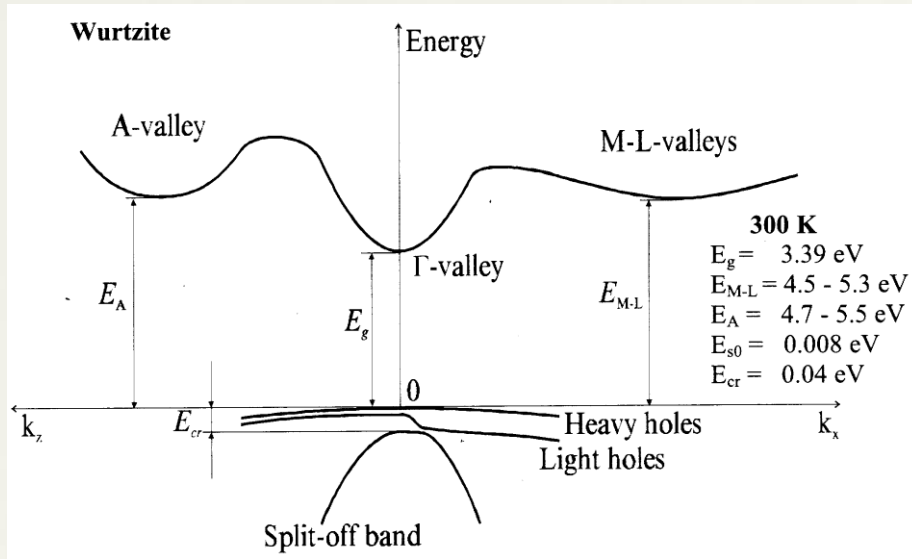
Guangle Zhou, Zongyang Hu  
Yeqing Lu, Jia Guo  
091123

# Outline

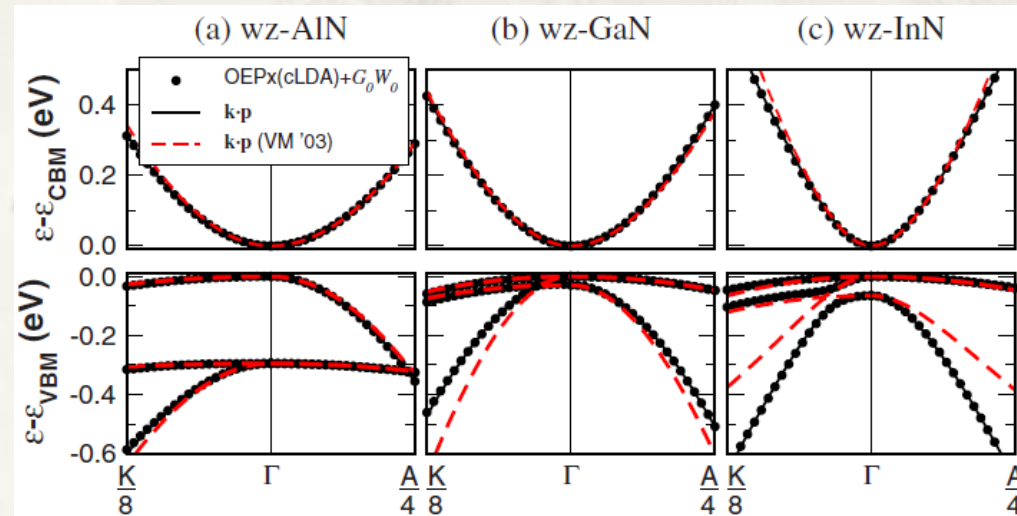
---

- \* Background and motivations
- \* AlN and InN band structure calculations by  $\vec{k}\cdot\vec{p}$
- \* Strain effect on the AlN and InN valence band and optical properties
- \* Quantum well confinement and strain effect on  $\text{In}_x\text{Al}_{1-x}\text{N}$  with different Al composition
- \* Conclusions and future work

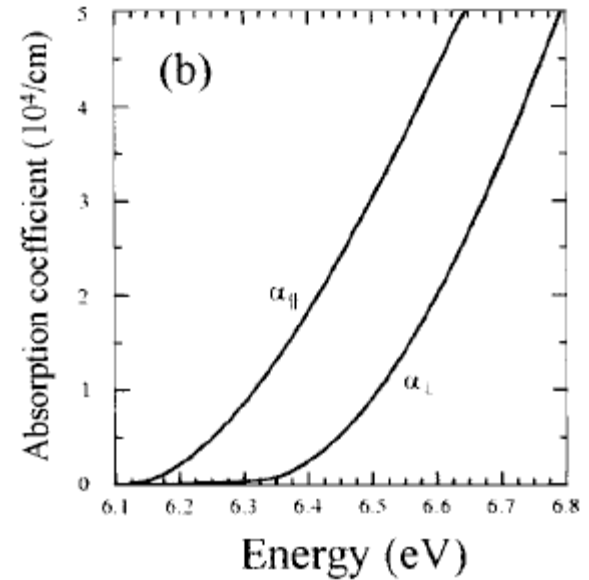
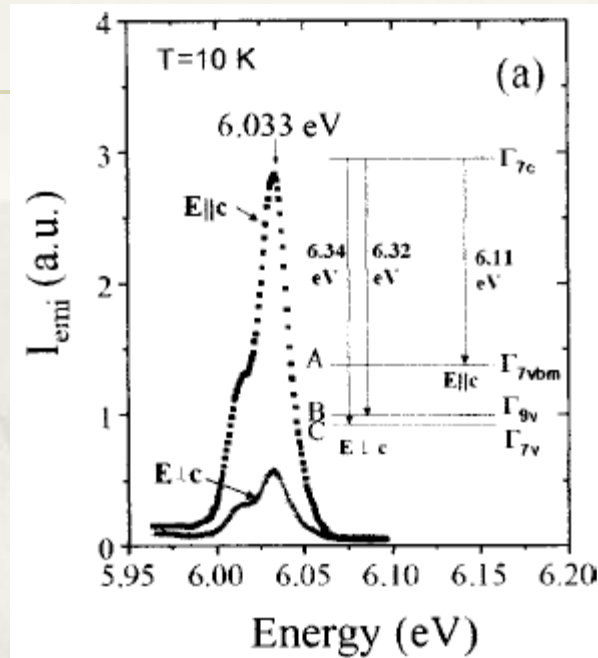
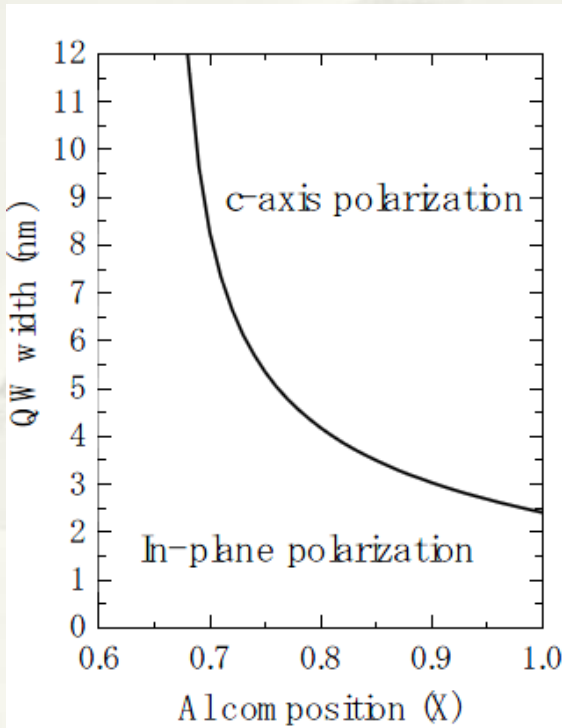
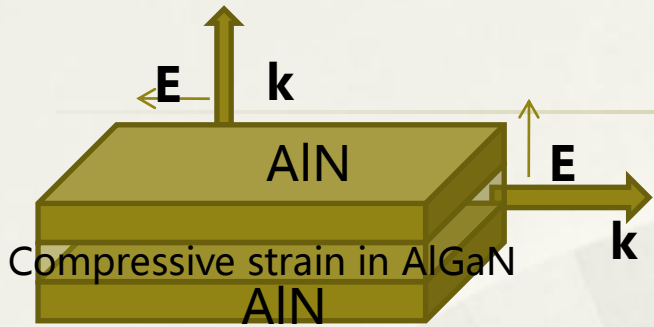
# III-V nitride band structures



## Band structure of wz-GaN(ioffe)



# Valence band engineering of III-V nitride



*PL Spectra of AlN on(0001) plane*

$E_{\parallel c}$  has much larger emission intensity than  $E_{\perp c}$   
**Related to Valence band structures of AlN!**

The valence band structure and light polarization can be modified by introducing strain effect and quantum confinement.

*Ref. Phys. Stat.sol(c), No.6, 2364-2366, 2007*  
*Ref. Appl. Phys. Lett., Vol. 83, No. 25, 22, 2003*

# $\vec{k} \cdot \vec{p}$ method for Band structure calculations

$$Hu_{n\mathbf{k}}(\mathbf{r}) \simeq \left( H_0 + \frac{\hbar^2 k^2}{2m_0} + \frac{\hbar}{m_0} \mathbf{k} \cdot \mathbf{p} + H_{so} \right) u_{n\mathbf{k}}(\mathbf{r})$$

$$= E_n(\mathbf{k}) u_{n\mathbf{k}}(\mathbf{r}),$$

$$H' = \begin{bmatrix} F & K_t & -iH_t & 0 & 0 & 0 \\ K_t & G & \Delta - iH_t & 0 & 0 & 0 \\ iH_t & \Delta + iH_t & \lambda & 0 & 0 & 0 \\ 0 & 0 & 0 & F & K_t & iH_t \\ 0 & 0 & 0 & K_t & G & \Delta + iH_t \\ 0 & 0 & 0 & -iH_t & \Delta - iH_t & \lambda \end{bmatrix}$$

$$E_1^0 = \Delta_1 + \Delta_2 + \theta_\epsilon + \lambda_\epsilon,$$

$$E_2^0 = \frac{\Delta_1 - \Delta_2 + \theta_\epsilon}{2} + \lambda_\epsilon + \sqrt{\left( \frac{\Delta_1 - \Delta_2 + \theta_\epsilon}{2} \right)^2 + 2\Delta_3^2},$$

$$E_3^0 = \frac{\Delta_1 - \Delta_2 + \theta_\epsilon}{2} + \lambda_\epsilon - \sqrt{\left( \frac{\Delta_1 - \Delta_2 + \theta_\epsilon}{2} \right)^2 + 2\Delta_3^2}.$$

Ref. S.L.Chuang, PRB, Vol 54, No.4, 1996

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

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

$$\lambda = \frac{\hbar^2}{2m_0} [A_1 k_z^2 + A_2 (k_x^2 + k_y^2)] + \lambda_\epsilon$$

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

$$\theta = \frac{\hbar^2}{2m_0} [A_3 k_z^2 + A_4 (k_x^2 + k_y^2)] + \theta_\epsilon$$

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

$$K = \frac{\hbar^2}{2m_0} A_5 (k_x + ik_y)^2 + D_5 \epsilon_+,$$

$$H = \frac{\hbar^2}{2m_0} A_6 k_z (k_x + ik_y) + D_6 \epsilon_{z+},$$

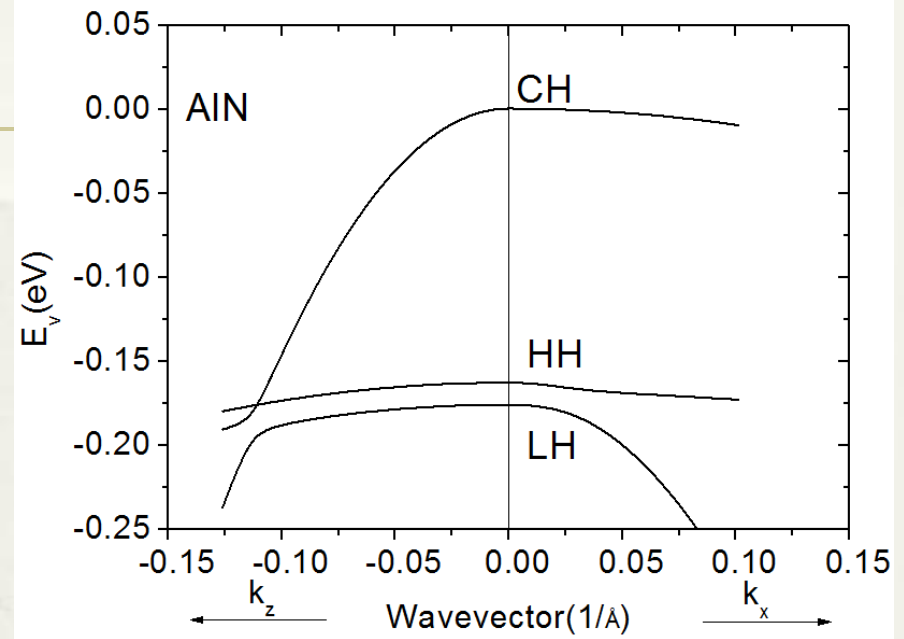
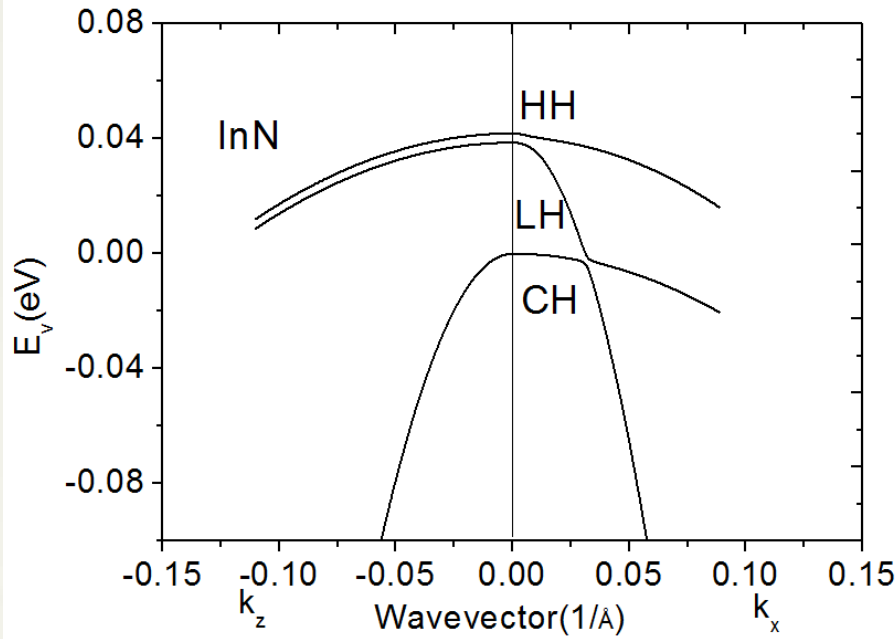
$$\Delta = \sqrt{2} \Delta_3,$$

where

Strain tensor:  $\epsilon_{\pm} = \epsilon_{xx} \pm 2i\epsilon_{xy} - \epsilon_{yy},$

$$\epsilon_{z\pm} = \epsilon_{zx} \pm i\epsilon_{yz}.$$

# Unstrained AlN and InN valence band structures



**AlN energy at  $\Gamma$  point (eV):**

$$E_{C\Gamma} = E_g(6.25) + E_{CH\Gamma}$$

$$E_{CH\Gamma} = 4.56e-04$$

$$E_{HH\Gamma} = -0.163$$

$$E_{LH\Gamma} = -0.176$$

**InN energy at  $\Gamma$  point (eV):**

$$E_{C\Gamma} = E_g(0.78) + E_{HH\Gamma}$$

$$E_{HH\Gamma} = 0.0417$$

$$E_{LH\Gamma} = 0.0385$$

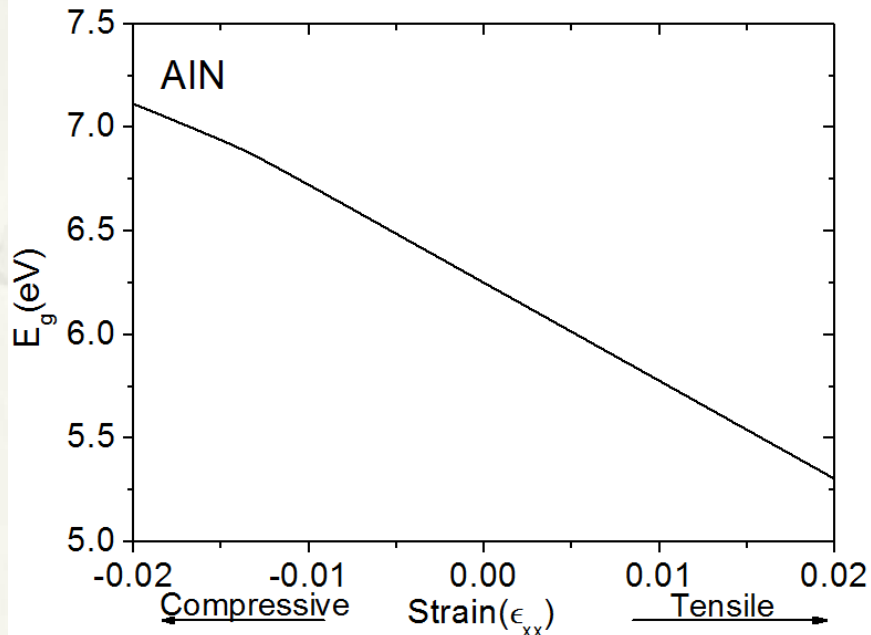
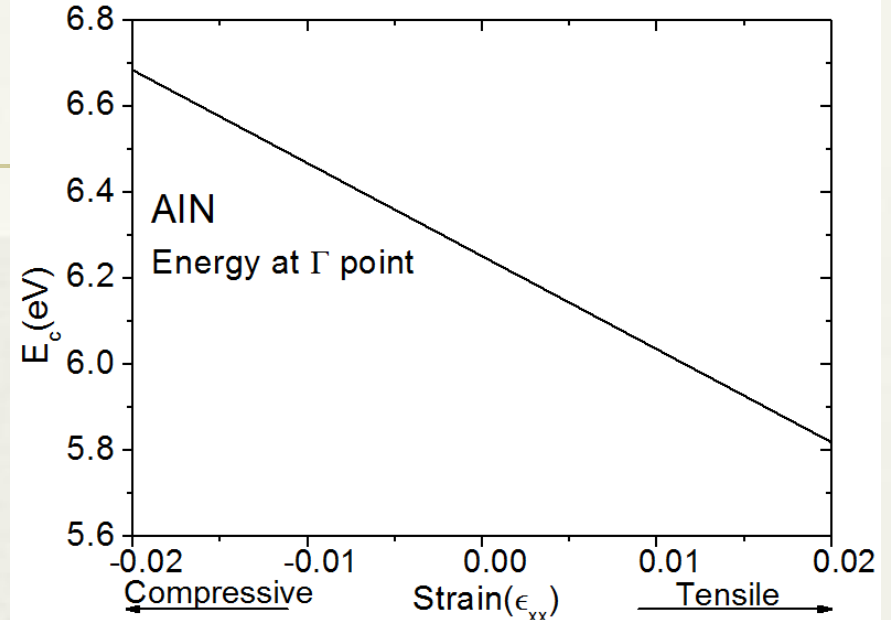
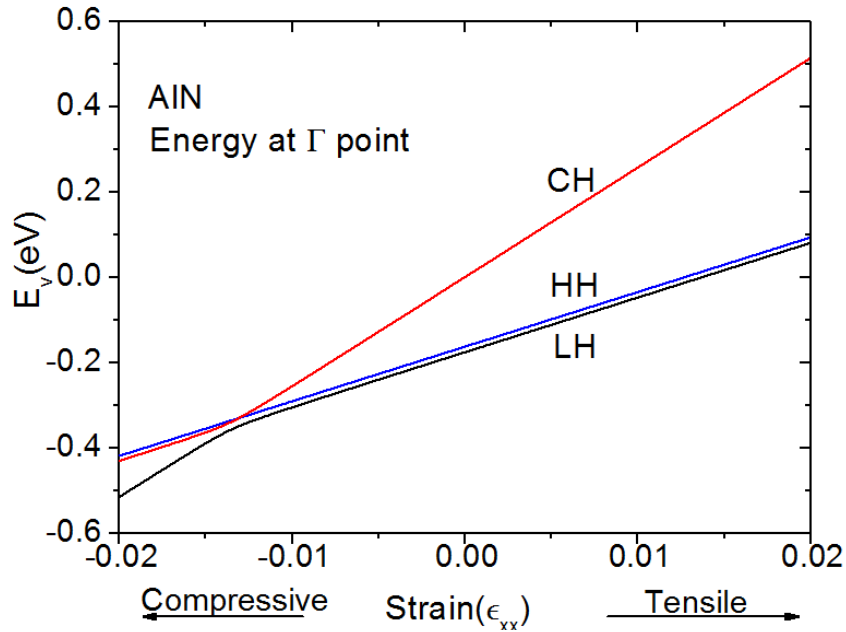
$$E_{CH\Gamma} = -1.44e-04$$

$$E_1 = F,$$

$$E_2 = \frac{G+\lambda}{2} + \sqrt{\left(\frac{G-\lambda}{2}\right)^2 + \Delta^2}$$

$$E_3 = \frac{G+\lambda}{2} - \sqrt{\left(\frac{G-\lambda}{2}\right)^2 + \Delta^2}$$

# Strained AlN valence band structures



Important parameters for AlN:

Strain tensor:

$$\epsilon_{xx} = \epsilon_{yy} = \frac{a_0 - a}{a}$$

$$\epsilon_{zz} = -\frac{2C_{13}}{C_{33}} \epsilon_{xx}$$

$a = 3.112 \text{ \AA}$

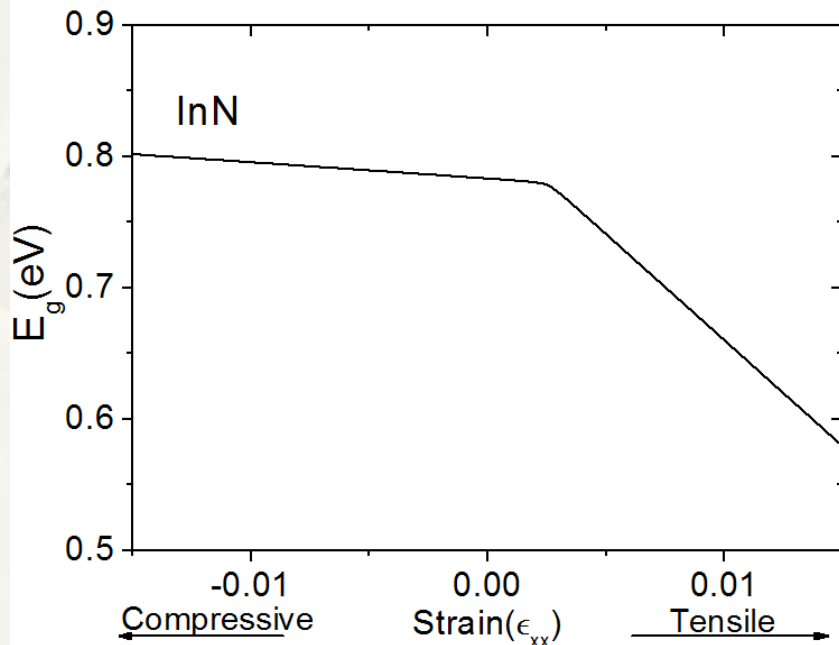
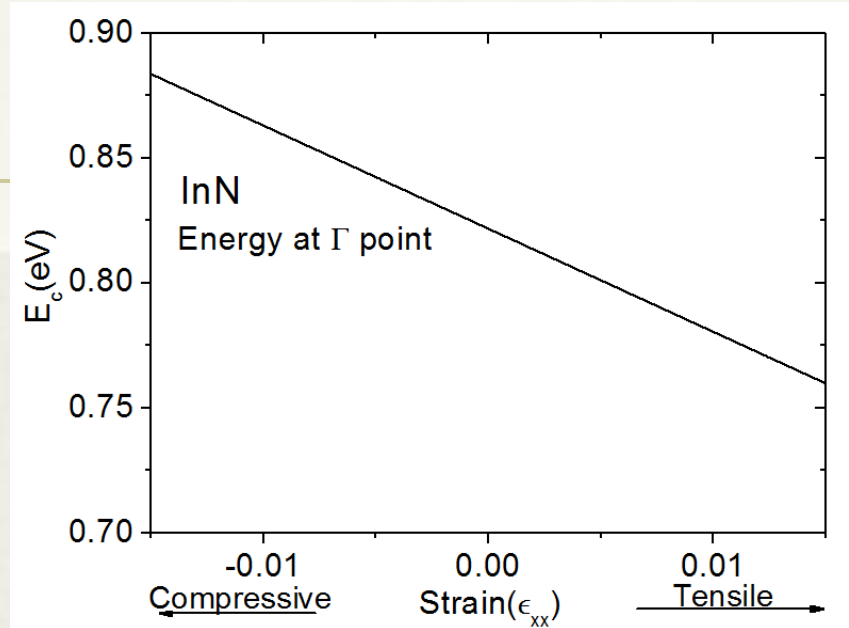
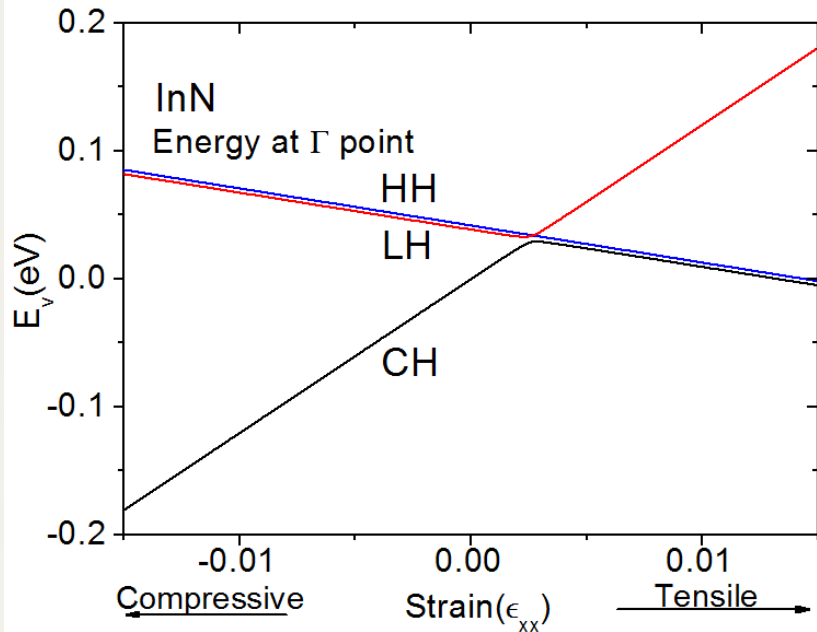
$C_{13} = 108 \text{ GPa}$

$C_{33} = 373 \text{ GPa}$

$\Delta_{cr} = 169 \text{ meV}$

$\Delta_{so} = 19 \text{ meV}$

# Strained InN valence band structures



Important parameters for InN:

$$a=3.543\text{\AA}$$

$$C_{13}=92\text{GPa}$$

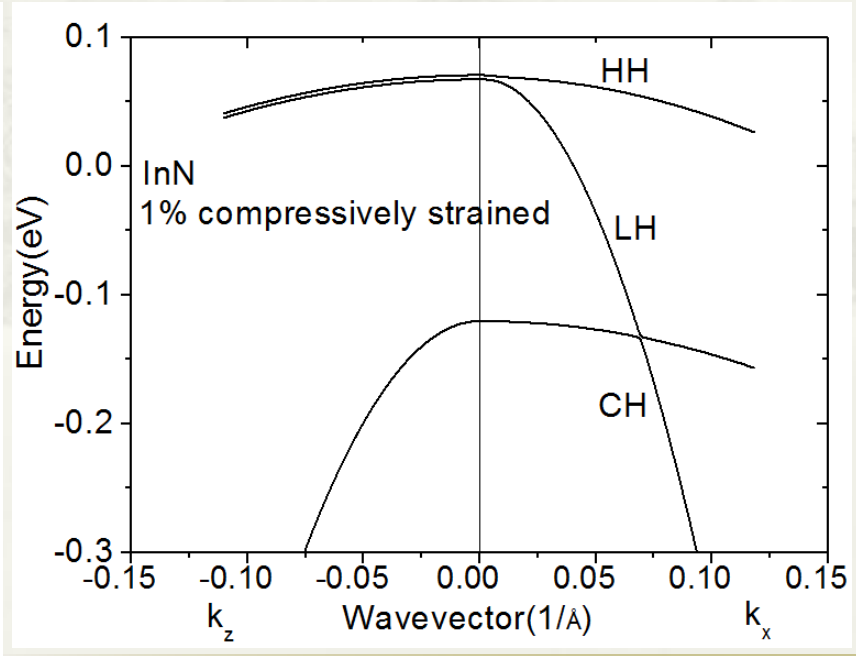
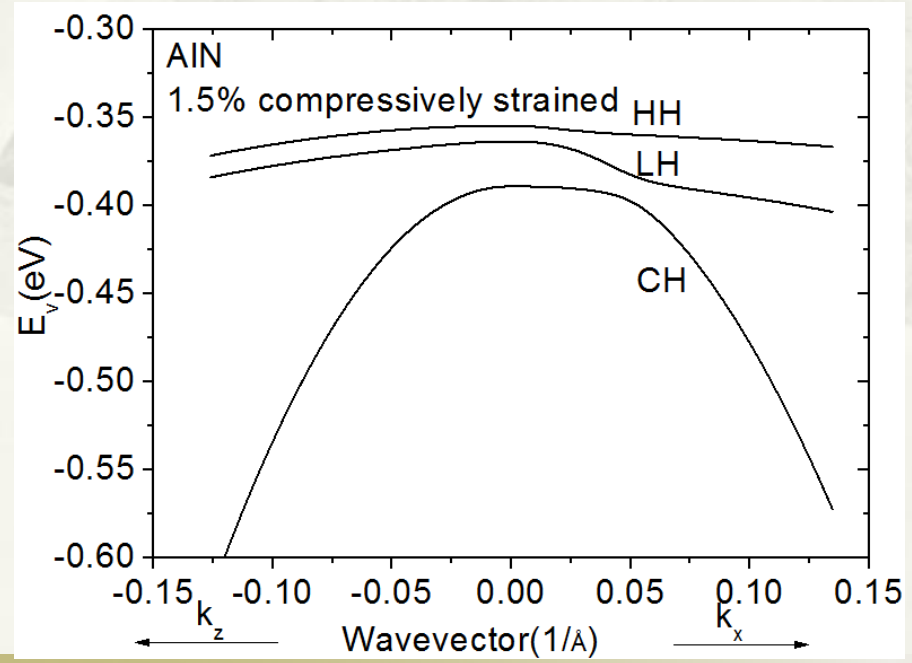
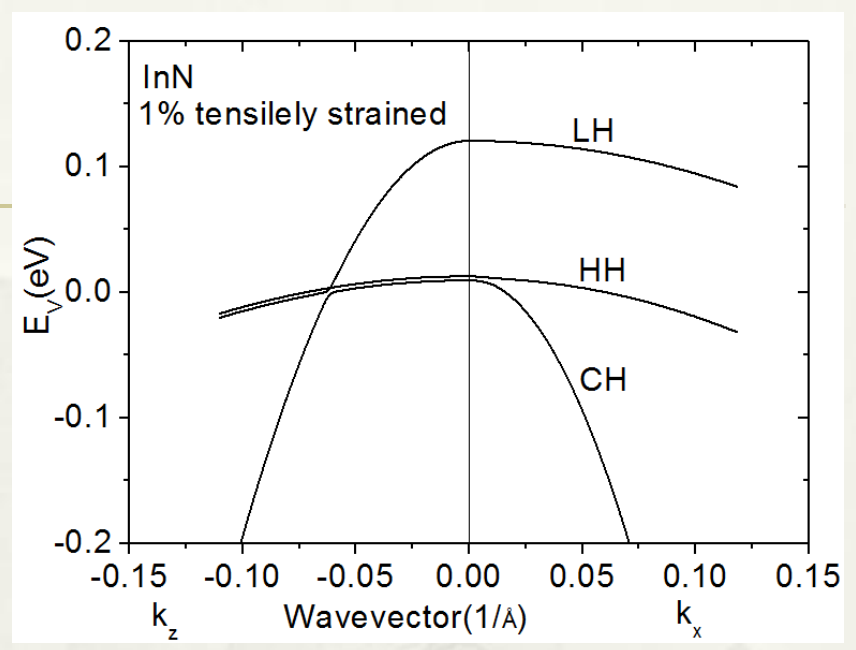
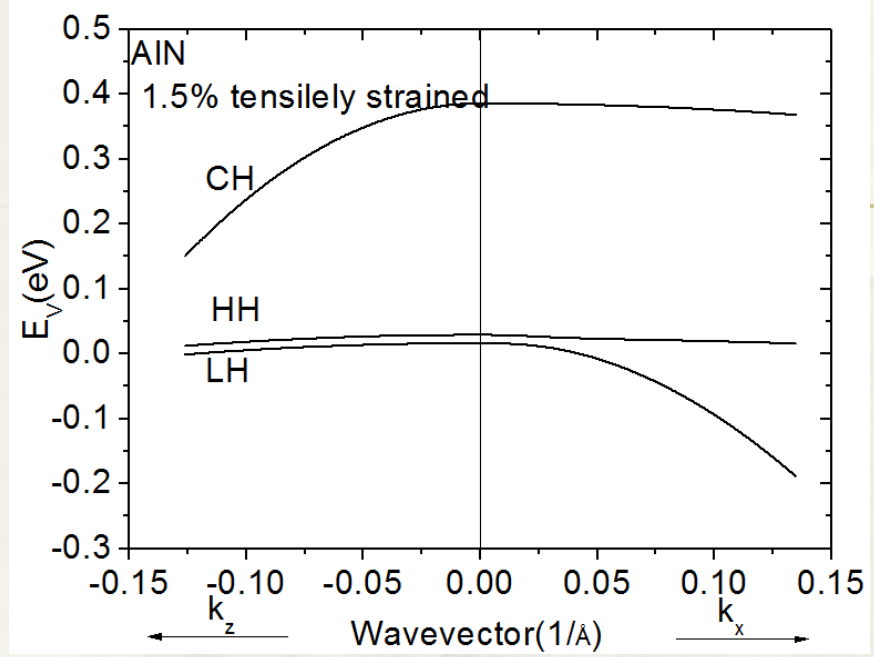
$$C_{33}=224\text{GPa}$$

$$\Delta_{cr}=40\text{meV}$$

$$\Delta_{so}=5\text{meV}$$

Here consider a strained-layer wurtzite crystal pseudomorphically grown along the (0001) (z axis direction)

# Strain effect on AlN and InN Valence band



# Strain effect on optical transition properties

Valence energy			$\hat{e} \parallel c$ axis	$\hat{e} \perp c$ axis
AlN	InN			
$E_1$	HH	HH	0	$\frac{m_0}{4} E_{px}$
$E_2$	CH	LH	$b^2 \left( \frac{m_0}{2} E_{pz} \right)$	$a^2 \left( \frac{m_0}{4} E_{px} \right)$
$E_3$	LH	CH	$a^2 \left( \frac{m_0}{2} E_{pz} \right)$	$b^2 \left( \frac{m_0}{4} E_{px} \right)$
Sum			$\frac{m_0}{2} E_{pz}$	$\frac{m_0}{2} E_{px}$

Use transition matrix elements to estimate:

$$|M|^2 = |\langle C | \vec{P} | \text{hole} \rangle \cdot \vec{e}|^2$$

$$|c \rangle = |iS \uparrow \rangle \quad |LH \rangle = a \times u_2 + b \times u_6$$

$$|HH \rangle = u_1 \quad |CH \rangle = b \times u_2 - a \times u_6$$

$$u_1 = -\frac{1}{\sqrt{2}} |(X + iY) \uparrow \rangle$$

$$u_2 = \frac{1}{\sqrt{2}} |(X - iY) \uparrow \rangle$$

$$u_6 = |Z \downarrow \rangle$$

$$E_{pz} = (2m_0 / \hbar^2) P_1^2 E_{px} = (2m_0 / \hbar^2) P_2^2$$

$$P_1^2 = \frac{\hbar^2}{2m_0} \left( \frac{m_0}{m_e^*} - 1 \right) \frac{(E_g + \Delta_1 + \Delta_2)(E_g + 2\Delta_2) - 2\Delta_3^2}{(E_g + 2\Delta_2)}$$

$$P_2^2 = \frac{\hbar^2}{2m_0} \left( \frac{m_0}{m_e^*} - 1 \right) \frac{E_g [(E_g + \Delta_1 + \Delta_2)(E_g + 2\Delta_2) - 2\Delta_3^2]}{(E_g + \Delta_1 + \Delta_2)(E_g + \Delta_2) - \Delta_3^2}$$

$$a^2 = \frac{E_2^0 - \lambda_\epsilon}{E_2^0 - E_3^0}, \quad b^2 = \frac{E_3^0 - \lambda_\epsilon}{E_3^0 - E_2^0}$$

Unstrained AlN:

$$E_2 = 4.56 \times 10^{-4} \text{ eV}$$

$$E_3 = -0.176 \text{ eV}$$

$$a^2 \sim 0.0026$$

$$b^2 \sim 0.9974$$

Unstrained InN:

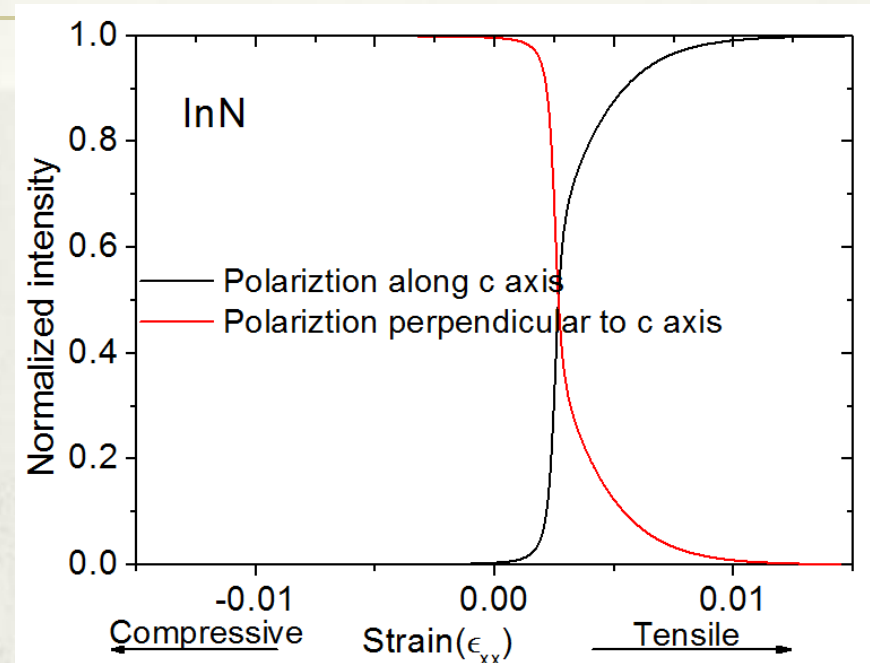
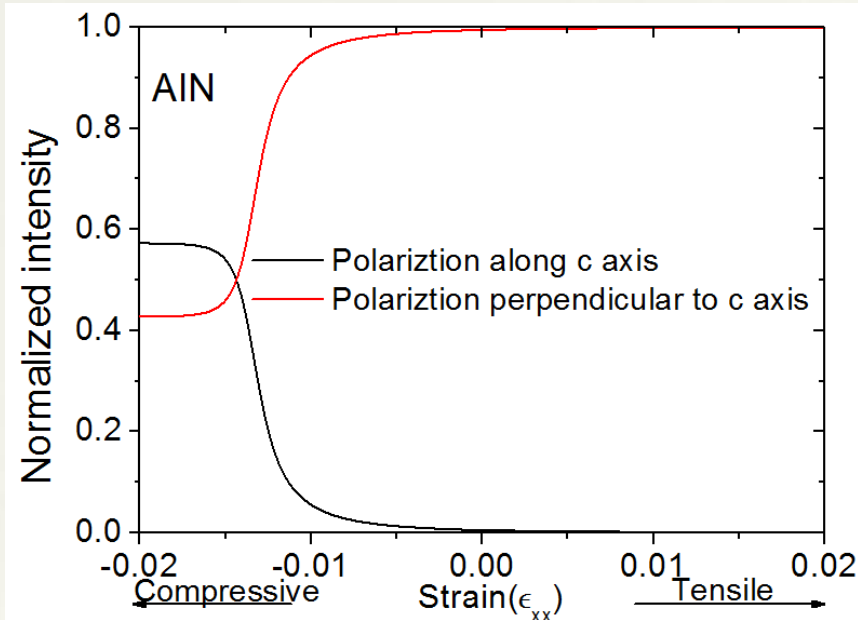
$$E_2 = 0.0385 \text{ eV}$$

$$E_3 = -1.44 \times 10^{-4} \text{ eV}$$

$$a^2 \sim 0.9963$$

$$b^2 \sim 0.0037$$

# Strain effect on AlN and InN optical transition properties



Consider two top bands:

- (1) AlN CH&HH Band
- (2) InN HH&LH Band

*Assumptions(??):*

$$I_{\text{total}} = I_{\text{top}} + \exp((E_{\text{bottom}} - E_{\text{top}})/kT) * I_{\text{bottom}}$$

Only top valence band considered!  
AlN/AlInN quantum well used.

Analytical solution of 6X6  
matrix:

$$E_1 = F$$

HH:

$$E_2 = \frac{G + \lambda}{2} + \sqrt{\left(\left(\frac{G - \lambda}{2}\right)^2 + \Delta^2\right)}$$

LH:

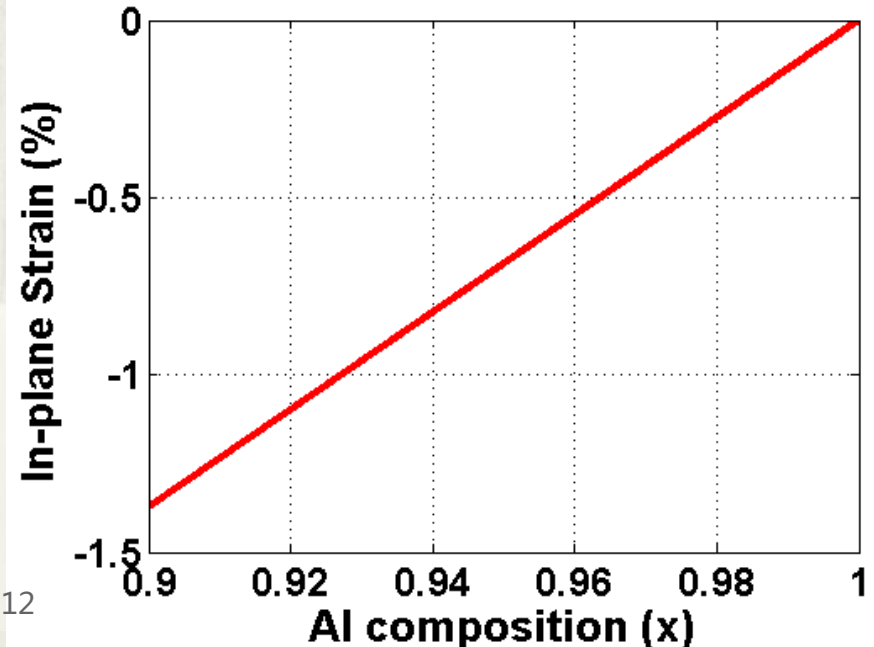
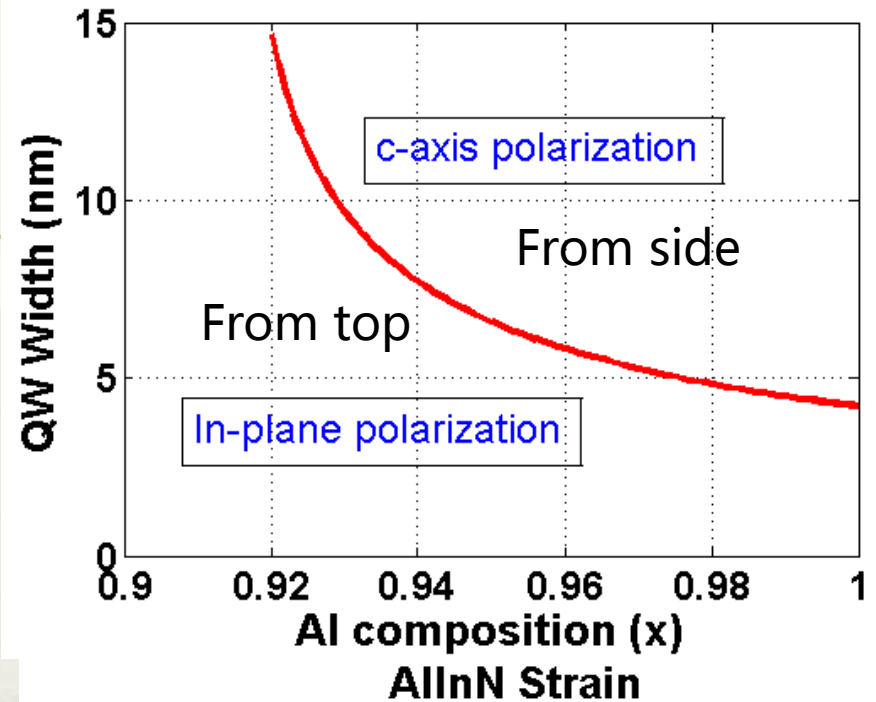
$$E_3 = \frac{G + \lambda}{2} - \sqrt{\left(\left(\frac{G - \lambda}{2}\right)^2 + \Delta^2\right)}$$

When  $E_3 > E_1$ , get Phase diagram:

$$|A_1| \cdot \left(\frac{\pi}{L}\right)^2 + \left(2 \frac{C_{13}}{C_{33}} + 1\right) \cdot D_4 C_{11} > -\frac{\Delta_{cr}}{2}$$

For this calculation, strain effect on  $m_z$   
At  $k=0$  was not included, that would  
effect the quantum effected energy  
split.

AllnN Phase diagram



# Conclusions

- \* Unstrained AlN and InN have different valence band structures, AlN has valence bands(CH HH LH) and InN valence bands(HH LH CH)
- \* Different strain effect can caused different valence band structures. For AlN  $>1.2\%$  compressively strain can change the top band from CH to HH. For InN  $>0.3\%$  tensilely strain can switch top band from HH to LH. Therefore, the optical proprieties are also changed by strain effects.
- \* Al composition has to be larger than 0.9 in order to have the polarization switch from the phase diagram, which is mostly due to the large lattice mismatch between AlN and InN.

# Future work

---

- \* P type doping
- \* Write up