Anisotropy of the Γ-point electron effective mass in hexagonal InN

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Aim

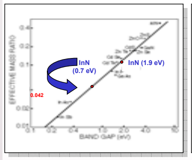
Experimental evidence for α-InN Γ-point effective electron mass value for polarization perpendicular to c-axis:

$m^*_{\perp}$ (k = 0) = 0.047 m_0

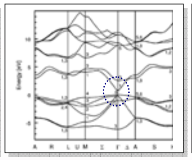
… increasing mass anisotropy towards lower Fermi energies, with approximately 17% smaller mass for polarization parallel to c-axis at *N* = 1.8x10^{17}cm^{-3}

Linear decrease of mobility in the double-Log(N) plot with better mobility parallel c-axis ($\mu_{\parallel} > \mu_{\perp}$) tentatively assigned to ionized impurity and boundary defect scattering

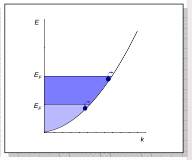
Motivation



Experimental and theoretical evidence for E_g(InN)~0.7eV – Γ-point effective mass has been overestimated!



Anisotropic Γ-point effective mass predicted by empirical pseudopotential calculations



Non-parabolic conduction band – effective mass depends on the free-charge-carrier concentration

B.R.Nag Phys. Stat. Sol. (b) **237**, R1 (2003)

D. Fritsch et al. PR **B 69**,165204(2004); P. Carrier and S.-H. Wei JAP 97 (2005)

$m^* = \hbar\left(\frac{\partial^2 E}{\partial k^2}\right)^{-1} \neq m^* = \hbar\left(\frac{\partial^2 E}{\partial k^2}\right)^{-1}$

Γ-point effective mass and anisotropy not determined experimentally!

Far-infrared Magneto-optic Generalized Ellipsometry:

contactless, non-destructive determination of phonon and free-charge-carrier parameters (concentration, effective-mass, mobility) in thin layer samples by stratified dielectric model calculation:

Free-charge-carrier effects

$$\varepsilon(\omega,\mathbf{H}) = -\langle\omega_p^{*2}\rangle\left[(\omega^2\mathbf{I}+i\omega\boldsymbol{\gamma}) - i\begin{pmatrix}0 & -h_3 & h_2\\ h_3 & 0 & -h_1\\ -h_2 & h_1 & 0\end{pmatrix}\langle\omega_c\rangle\right]^{-1}$$

$\langle\omega_c\rangle = q\left(\frac{H}{m_e}\right)\mathbf{m}^{-1}$ Cyclotron (frequency) tensor

$\langle\omega_p^{*2}\rangle = N\frac{e^2}{m_e}\mathbf{m}^{-1}$ Plasma (frequency) tensor

Electronic contribution

Polar lattice contribution

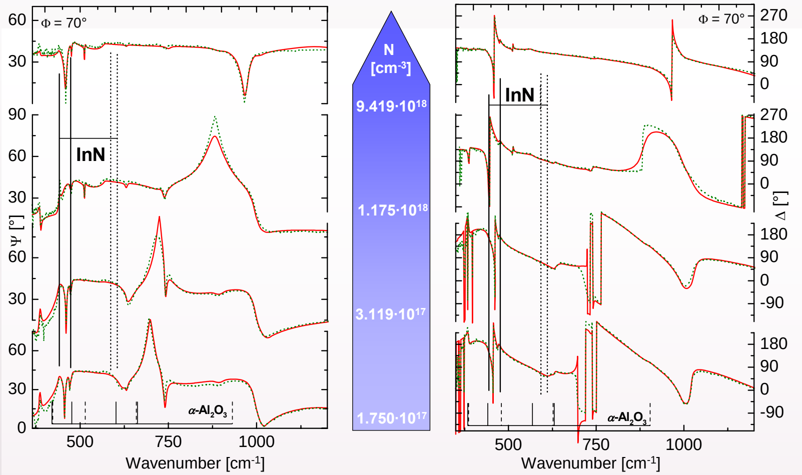
$$\varepsilon_j(\omega) = \varepsilon_{\infty,j}\cdot\prod_{i=1}^{l}\frac{\omega^2+i\gamma_{LO,ij}\omega-\omega^2_{LO,ij}}{\omega^2+i\gamma_{TO,ij}\omega-\omega^2_{TO,ij}}$$

Infrared-active phonon modes

Recent publications on MO generalized ellipsometry:

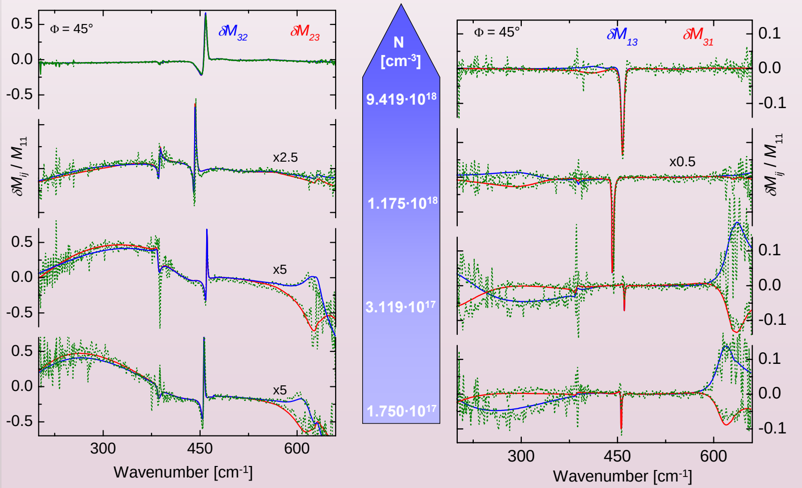
T. Hofmann et al. Rev. Sci. Instrum. **77**, 063902 (2006)
M. Schubert et al. Thin Solid Films **455-456**, 563-570 (2004)
T. Hofmann et al. Mat. Res. Soc. Symp. Proc. **744**, M5.32.1-6 (2003)
T. Hofmann et al. Appl. Phys. Lett. **82**, 3463-3465 (2003)
M. Schubert et al. J. Opt. Soc. Am. A **20**, 347-356 (2003)

Standard Ellipsometry (Zero-Magnetic-Field): Psi and Delta



Zero-Field Standard Ellipsometry spectra reveal thickness, phonon mode frequency and broadening parameters, static dielectric constants, plasma frequency and plasma broadening parameters of InN and GaN layers upon model layer calculations

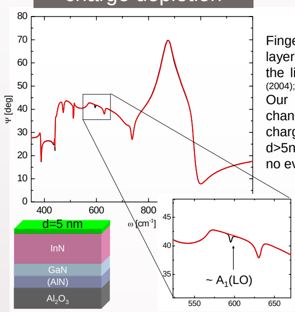
Magneto-optic Generalized Ellipsometry: Mueller Matrix



The spectra above are differences between Mueller matrix data (chiral elements M_{13}, M_{31}, M_{32}, and M_{23}) measured magnetic fields of +4.5T and -4.5T. The non-chiral elements M_{12}, M_{21}, M_{22}, and M_{33} vanish. Vertical solid and dashed lines within the Standard Ellipsometry spectra indicate the TO and LO mode frequencies, of the InN film and the sapphire substrate.

Results and Discussion

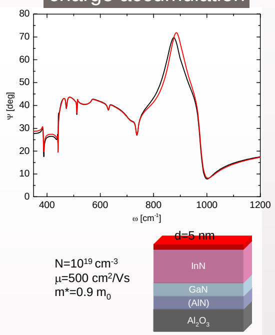
charge depletion



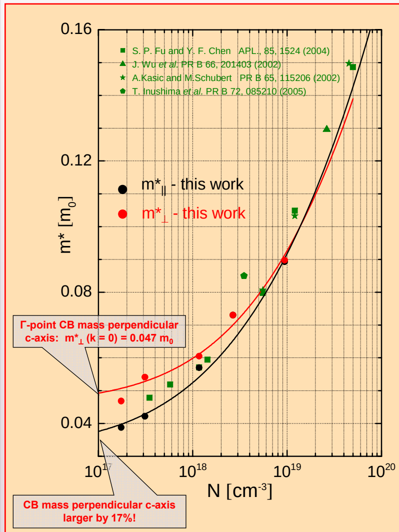
Fingerprints of a thin carrier accumulation layer in wurzite InN have been reported in the literature. PR B **69**, 201307(R) (2004); JCG **269**, 29 (2004); PRL **92**, 036804 (2004); APL **82**, 1736 (2003)

Our model calculations show distinct changes in the ellipsometric spectra if a charge depletion or accumulation layer d>5nm would be present, but experimentally no evidence of such a layer was observed.

charge accumulation



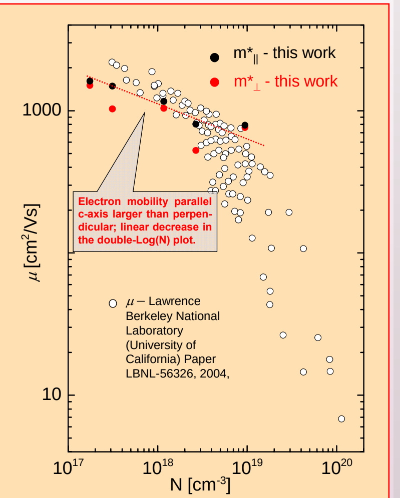
Anisotropy of α-InN Γ-point CB-electron mass and mobility



Application of Kane's two-band model:

$0.047 = m^*_{\perp} > m^*_{\parallel} = 0.039$

Kane's two-band model suggests:
Eg (E ⊥ c) = 0.7 eV
Eg (E ∥ c) = 0.4 eV



Anisotropy corresponds with recent LDA-corrected calculations (P.Carrier and S-H. Wei JAP 97 (2005):

Calculated: 14 %
this-work: 17 %

ICPS, 24.-28. July, 2006

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