Lattice modes and free-carrier response of $Al_xGa_{1-x}N$ and $In_xGa_{1-x}N$ heterostructures and strained GaN-AlN-superlattices measured by infrared ellipsometry

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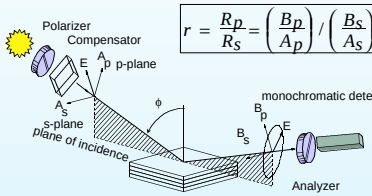
Outline

We determine the anisotropic dielectric functions of wurtzite III-N materials grown by MOCVD or MBE on (0001) sapphire using spectroscopic ellipsometry (SE) within the infrared (IR) spectral range [333 cm^{-1} (30 µm) ... 3333 cm^{-1} (3 µm)].

We present phonon-mode frequencies and free-carrier parameters in:
- Si-doped *n*-type and Mg-doped *p*-type *a*-GaN
- *a*-$Al_xGa_{1-x}N$ ($0<x<1$) and *a*-$In_xGa_{1-x}N$ ($x<0.3$)
- strained GaN-AlN superlattice structure.

We discuss energy-dependence of electron and hole effective mass in *a*-GaN, and strain in *a*-GaN-AlN-SL structure.

Spectroscopic ellipsometry (SE)



$$r = \frac{R_p}{R_s} = \left(\frac{B_p}{A_p}\right) / \left(\frac{B_s}{A_s}\right) = \tan\Psi e^{i\Delta}$$

Ellipsometry measures the ratio of R_p vs. R_s [Azzam-89] in terms of Ψ and Δ. Model calculations are performed until measured and calculated data match as closely as possible [Jellison-98]. The mean-square error function employed is weighted to the experimental errors [Herzinger-95].

III-Nitride dielectric function model

A factorized model [Gervais-74] is employed for the lattice contribution. The Drude approximation is used to calculate the free-carrier response [Wolfe-89].
LO, TO phonons, and broadening parameters: w_{LO}, w_{TO}, g_{TO}, g_{LO}.
Polarization perpendicular to the *c*-axis : (E_1)-modes
Polarization parallel to the *c*-axis : (A_1)-modes. See, e.g., [Orton-98].

lattice contribution (FPSQ model) | free-carrier absorption (Drude model)

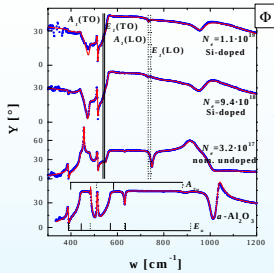
$$\epsilon_j = \epsilon_{\infty j} \prod_i^l \frac{w_{LOi}^2 - w^2 - iwg_{LOi}}{w_{TOi}^2 - w^2 - iwg_{TOi}} + i\frac{e^2 n}{m_j^* \epsilon_0 w}\left\langle t_m^* \right\rangle_j \Big|_{j=\parallel,\perp}$$

The effective mass m^*_j and the energy-averaged carrier momentum life time $\langle t^*_m \rangle$ are anisotropic. $\langle t_m \rangle$ is substituted by the optical carrier mobility m_j.

$$\left\langle t_m^* \right\rangle_j = \left\langle t^m \left(1 - iwt^m\right)^{-1} \right\rangle_j = \left\langle t^m \right\rangle_j \left\langle 1 - iwt^m \right\rangle_j^{-1} \Big|_{j=\parallel,\perp}$$

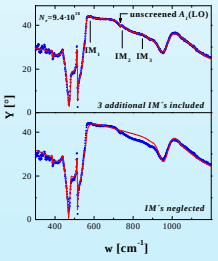
$$\langle t_m \rangle_j = \left(m_j^* / e\right) m_j \Big|_{j=\parallel,\perp}$$

n-type *a*-GaN/*a*-Al_2O_3



IR-SE provides high sensitivity to the frequencies and broadening values of the IR-active E_1(TO), A_1(LO) and E_1(LO) *a*-GaN lattice modes. High free-electron concentrations cause enormous changes in the IR-SE spectra compared to low-conductive films.

Impurity modes & depletion layer



⇒ 3 ***IR-active***, but ***Raman-inactive*** impurity modes with ***small TO-LO splitting values*** occur in highly Si-doped *n*-type *a*-GaN:

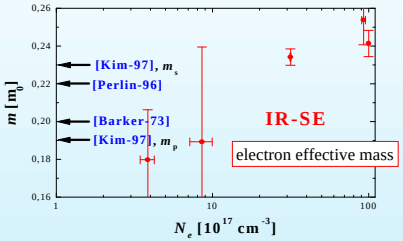
IM_1: **569±5** cm^{-1} ⇒ disorder-activated $E_2^{(2)}$
IM_2: **747±5** cm^{-1} ⇒ ?
IM_3: **855±8** cm^{-1} ⇒ ac.-optical combination

⇒ An approx. 10 nm thick carrier-depleted *a*-GaN layer on the sample surface can be explained by Fermi-level pinning at surface states localized within the band gap.

Electron and hole effective mass in *a*-GaN

By performing the model based IR-SE data analysis we determine the *anisotropic*
- ***phonon frequencies and broadening values*** (⇒ layer strain and quality),
- ***dielectric function***,
- ***high-frequency dielectric constant***,
- ***the free-carrier parameter values (effective mass and carrier mobility)***, and

the layer thickness of the *a*-GaN layers.
Especially in the case of Si-doped *n*-type *a*-GaN we find a **dependence of the (isotropically averaged) effective mass on the carrier concentration** using the carrier Hall mobility as input parameter for our model calculations.



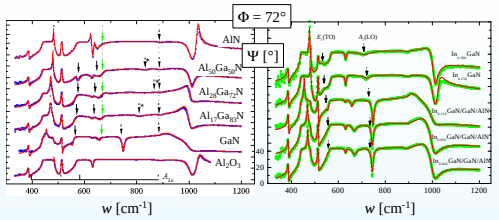
Because of small hole concentration ($N_h \le 3\cdot10^{18}$ cm^{-3}) and typical strong plasmon damping in *p*-type *a*-GaN, the determination of the free-hole parameter values is difficult. Nevertheless, **IR-SE provides** the hole mobility values as well as the **hole effective mass m_h without substantial anisotropy**.

N_h [cm^{-3}]	m_h [m_0]
$5\cdot10^{17}$	0.74±0.17
$8\cdot10^{17}$	1.40±0.33

hole effective mass

a-$Al_xGa_{1-x}N$

a-$In_xGa_{1-x}N$



IRSE (Ψ) data for *a*-$Al_xGa_{1-x}N$ and *a*-$In_xGa_{1-x}N$ heterostructures grown on *a*-Al_2O_3. The sapphire reststrahlen bands (A_{2u}, E_u) are present throughout all spectra, and those of a bare (0001) substrate are included for comparison (See Ref. [Schubert-PRB-00]). The *a*-$Al_xGa_{1-x}N$ spectra shown here reveal a two-(one) mode behavior for E⊥*c* (E||*c*), and are influenced by free carriers (See Ref. [Schubert-MRS-99]). The *a*-$In_xGa_{1-x}N$ spectra reveal a single mode behavior.

a-III-N phonon modes determined so far by IR-SE. For *a*-$Al_xGa_{1-x}N$ two IR-active E_1-modes are present for $0 < x < 1$.

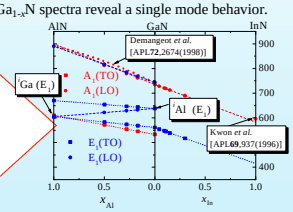
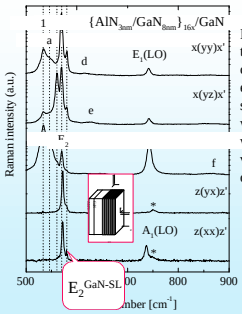


TABLE I: *a*-$Al_xGa_{1-x}N$ "impurity" modes ($x \to 0, 1$)

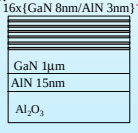
Impurity Mode			*i*GaN (E_1) ($x \to 1$)	*i*AlN (E_1) ($x \to 0$)
	substrate	*method*	[cm^{-1}]	[cm^{-1}]
[Schubert-MRS-99]	Al_2O_3	IR-ellipsometry	605	638
[Wisniewski-98]	6H-SiC	IR-reflectometry	622	643

µ-Raman



GaN-AlN-Superlattice

IR-SE (Ψ) data and µ-Raman spectra reveal additional SL-phonon modes similar to those observed in Ref. [Gleize-99]. The shift of the GaN-SL E_2 and E_1(TO) modes can be used to estimate the strain in the SL ([Davydov-97], [Tripathy-99]). Using elastic constants for GaN, the obtained stress (σ_{xx} ~ -4.5 GPa) is very similar to the strain induced by the SL-sublayers if a common in-plane lattice constant is adopted within the SL structure (σ_{xx}~-3.15 GPa). Furthermore, free-carriers (N_e~$8\cdot10^{18}$$cm^{-3}$) with assumed effective mass $0.22\cdot m_0$ are located within the GaN-sublayers. Their vertical (~32cm^2/(Vs)) and lateral (~320cm^2/(Vs)) mobility values differ by a factor of 10!

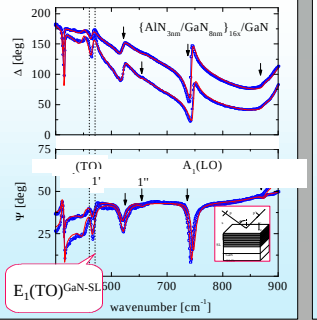


GaN-sublayer: N_e ~ $8\cdot10^{18}$ cm^{-3}
$m_\perp \sim 10\cdot m_\parallel \sim 320$ cm^2/(Vs)
⇒ vertical carrier confinement

SL-biaxial stress: σ_{xx} ~ -4.5 GPa
⇒ strained GaN-AlN-SL

E_2^{GaN-SL}

IRSE



$E_1(TO)^{GaN-SL}$

Conclusions

IR-SE is an excellent tool to determine lattice phonon mode frequencies and free-carrier parameters in III-N thin films.

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