IR-VUV Dielectric Function of $Al_{1-x}In_xN$ determined by Spectroscopic Ellipsometry

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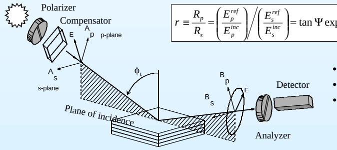
Introduction

We study the infrared to deep-ultra-violet optical response of MOVPE-grown **hexagonal $Al_{1-x}In_xN$** films for compositions $0.110 \le x \le 0.212$ using **Spectroscopic Ellipsometry**. $Al_{1-x}In_xN$ has prospects for application as confinement layer lattice matched to GaN and as active material for LED's and LD's operating in the NIR-VUV spectral range.

Summary

① Observation of one-mode behavior of the ir-active E_1(TO) phonon in contrast to theoretical predictions [1]
① Separation of alloying and in-plane strain effects on the observed E_1(TO) mode shift
② Detection of the A_1(LO) phonon mode
③ Measurement of fundamental band gap energy vs. alloy composition x
④ Measurement of NIR-VUV n and k spectra

Spectroscopic Ellipsometry



$$r \equiv \frac{R_p}{R_s} = \left(\frac{E_p^{ref}}{E_p^{inc}}\right) \Big/ \left(\frac{E_s^{ref}}{E_s^{inc}}\right) = \tan\Psi \exp(i\Delta)$$

- room temperature
- multiple angles of incidence
- rotating-compensator, Fourier-transform based mid-infrared spectroscopic ellipsometer

VASE®, IR-VASE™, VUV-VASE™, J.A. Woollam Co., Inc., Lincoln, NE

Data Analysis

Comparing measured and calculated data through regression data analysis: **lineshape fit**

⇨ **parameterized film dielectric function and film thickness**

mid-IR

$$\varepsilon^j(\omega) = \varepsilon_{\infty,j} \frac{\omega_{LO,j}^2 - \omega^2 - i\Gamma_j\omega}{\omega_{TO,j}^2 - \omega^2 - i\Gamma_j\omega} - \frac{\varepsilon_{\infty,j}\omega_{p,j}^2}{\ldots}$$

phonon properties | **free-carrier properties**

$j = \parallel, \perp$ c-axis

NIR-VUV

$$\varepsilon^j(\omega) = \varepsilon_{\infty,j} + \sum \frac{f_{k,j}\exp(i\varphi_{k,j})}{\omega_{k,j}^2 - \omega^2 - i\omega\Gamma_{k,j}\exp\ldots}$$

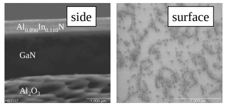
band-gap parameters

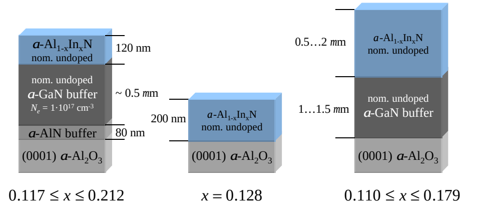
parameters

$\omega_{TO,j}$	TO frequency
$\omega_{LO,j}$	LO frequency
Γ_j	mode broadening
$\varepsilon_{\infty,j}$	high-frequency dielec. function limit
$\omega_{p,j}$	screened plasma frequency
$\gamma_{p,j}$	plasma broadening
$f_{k,j}$	k^{th} osc. amplitude
$\omega_{k,j}$	k^{th} osc. frequency
$\Gamma_{k,j}\cdot\exp[\ldots]$	k^{th} osc. broadening
$\varphi_{k,j}$	k^{th} osc. phase factor

Samples

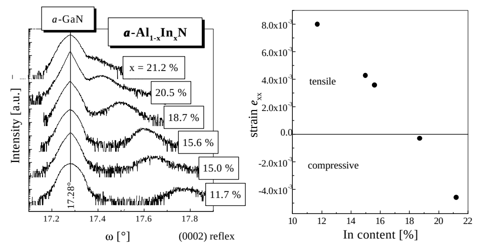
MOCVD, T_{gr} = 750° C
precursors: TMAl, TMIn, NH_3
University Stuttgart (Germany)





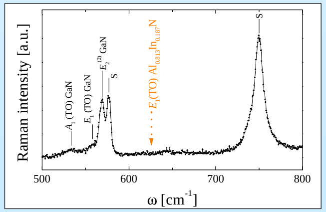
High-resolution XRD

$$e_{xx} = \frac{a_{exp}^{AlInN} - a_{rel}^{AlInN}}{a_{rel}^{AlInN}} - \frac{a_{exp}^{GaN} - a_{rel}^{GaN}}{a_{rel}^{GaN}}$$



Assuming Vegard's law, the composition x follows from the measured c- and a-lattice constants. a-$Al_{0.820}In_{0.180}N$ is expected to be lattice matched to strain-free a-GaN.

Raman Scattering



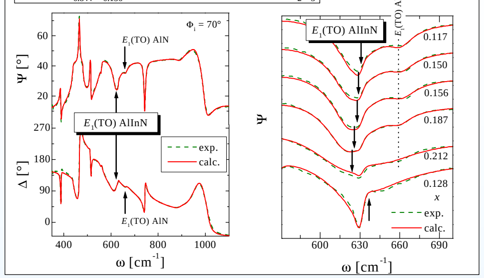
z(x,-)z´
λ_{ex} = 514.5 nm
P_{ex} = 100 mW

118 nm a-$Al_{0.813}In_{0.187}N$
561 nm a- GaN
84 nm a- AlN
a- Al_2O_3

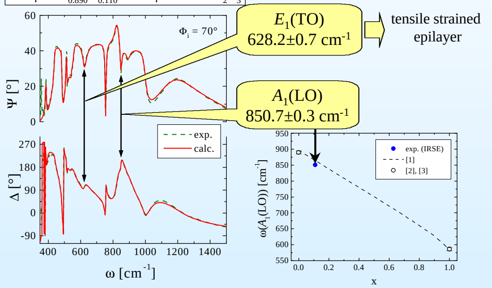
Micro-Raman scattering measurements do not reveal any $Al_{1-x}In_xN$ phonon modes for layer thicknesses $d \le 0.2$ mm.

Ellipsometry: ~ 300 ... 3000 cm^{-1}

118 nm $Al_{0.844}In_{0.156}N$ / 488 nm GaN / 76 nm AlN / Al_2O_3



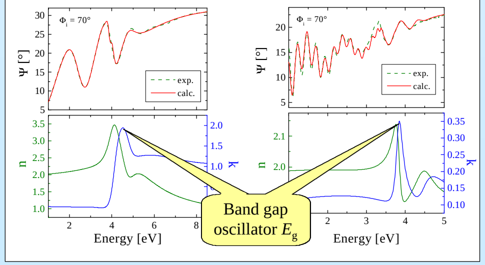
0.55 µm $Al_{0.890}In_{0.110}N$ / 1.5 µm GaN / Al_2O_3



Ellipsometry: ~1 eV … 8.5 eV

196 nm $Al_{0.872}In_{0.128}N$ / Al_2O_3

346 nm $Al_{0.827}In_{0.173}N$ / 882 nm GaN / Al_2O_3

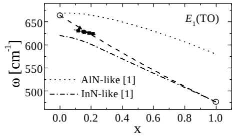


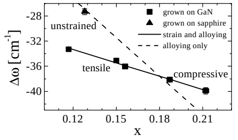
Results

1), 2): We observe a **one-mode behavior of the E_1(TO) phonon** in contrast to theoretical predictions using a MREI approach [1].
The observed $Al_{1-x}In_xN$ E_1(TO) mode shift Δω with respect to unstrained AlN is **induced by alloy composition x and film in-plane strain e_{xx}**:

$$\Delta\omega = \Delta\omega(x) + \Delta\omega(e_{xx}) = a_0 x + a_1 x(1-x) + b e_{xx}$$

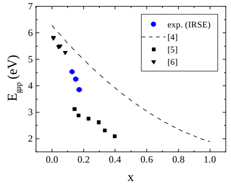
The ~120 nm thick $Al_{1-x}In_xN$ films are grown **pseudomorphically** on slightly strained GaN buffer layers.
The ~200 nm thick $Al_{1-x}In_xN$ film is grown **fully relaxed** directly on Al_2O_3.



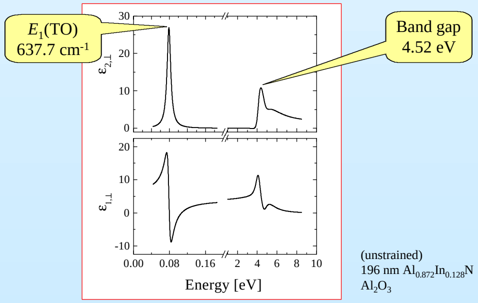


3): The ir-ellipsometry data reveal the **A_1(LO) phonon mode frequency at 850.7±0.3 cm^{-1}** for an unstrained $Al_{0.890}In_{0.110}N$ film.

4), 5): The $Al_{1-x}In_xN$ **fundamental band gap energies** as well as the **index of refraction and the absorption index** below and above the band gap were determined for different alloy compositions.



IR-VUV Dielectric Function



(unstrained)
196 nm $Al_{0.872}In_{0.128}N$
Al_2O_3

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