Strain relation in GaN nanowires with Al_2O_3 and HfO_2 shells examined by X-ray diffraction and Raman spectroscopy techniques

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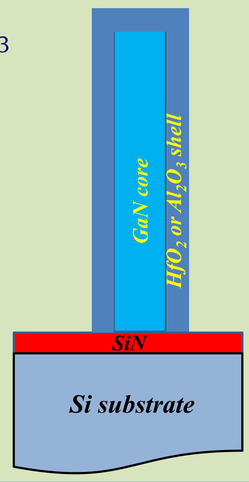
AIM OF THE WORK

- To check the strain relation between GaN core and oxide shells in nanowire system.
- To study the type of strain using X-ray diffraction techniques.
- To calculate the accurate values of lattice parameters of GaN core parts.
- To find the in-plane (ε_{xx}) and out-of-plane (ε_{zz}) strain values of GaN.
- To measure lattice vibration mechanisms, crystalline quality and in-plane (ε_{xx}) strain values by Raman spectroscopy.
- To compare strain relations obtained by XRD and Raman spectroscopy techniques.

GROWTH OF SAMPLES

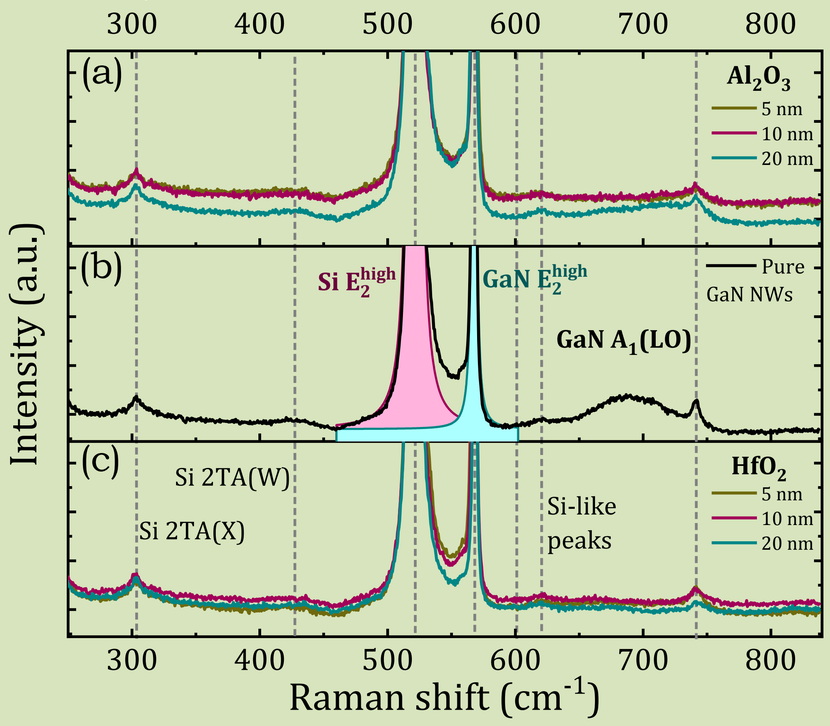
- GaN nanowires were grown catalyst-free on nitridated silicon (111) substrates by plasma-assisted molecular beam epitaxy (PAMBE) technique. On this GaN-core parts the following shell parts were grown:

- **SAMPLES A** - Al_2O_3 shell parts with different thicknesses: 5 nm (**A-5**), 10 nm (**A-10**) and 20 nm (**A-20**) were grown by atomic layer deposition (ALD) technique at low temperature.



- **SAMPLES H** – HfO_2 shell parts with different thicknesses: 5 nm (**H-5**), 10 nm (**H-10**) and 20 nm (**H-20**) were grown by ALD technique at low temperature.

μ-RAMAN SPECTROSCOPY



Non-resonant μ-Raman spectra of GaN-core and Al_2O_3-shell parts NWs (a) and GaN-core and HfO_2-shell parts NWs (c) compared to pure GaN NWs (b). The measurements were performed with excitation of 532 nm semiconductor laser.

- GaN E_2^{high} and GaN A_1(LO) phonon modes from GaN-core is observed.
- phonon modes are shifted with the oxide shell thickness.

CONCLUSIONS

- XRD measurements show good crystallographic quality of the GaN-core, oxide-shells NWs on Si(111) substrates.
- XRD 2θ/ω scans of 0002 GaN symmetrical reflection are shifted with the thickness of Al_2O_3 and HfO_2 shells.
- Accurate values of lattice parameters of GaN core were calculated from GaN 0002 symmetrical and GaN -1-124 asymetrical RSMs.
- Strain values in out-of-plane ε_{zz} and in-plane ε_{xx} direction were calculated from XRD measurements.
- μ-Raman spectra for samples with core-shell NWs were detected and compared with spectra for pure GaN NWs.
- Strain values in in-plane ε_{xx} direction were calculated from μ-Raman spectroscopy measurements.
- The values of in-plane direction ε_{xx} strain are similar from XRD and Raman spectroscopy and changes in the same way.

EXPERIMENTAL TECHNIQUES

X-ray diffraction (XRD):

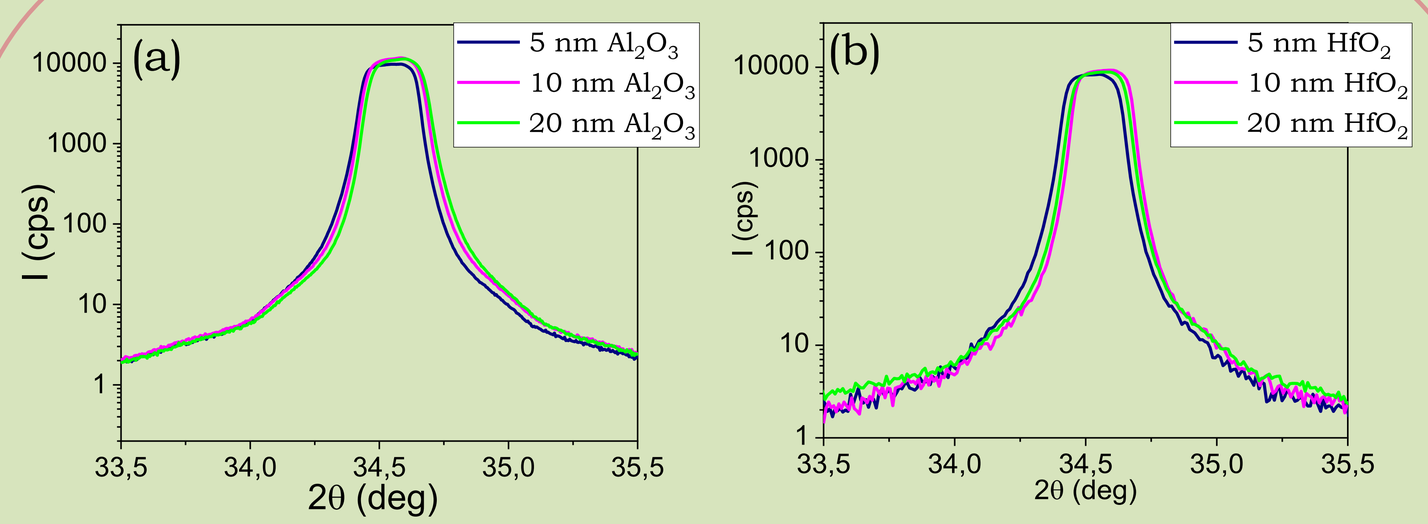
- X-ray diffraction measurements were performed using a Panalytical X'Pert Pro MRD diffractometer equipped with a lamp with CuKα1 radiation, a hybrid two-bounce Ge (220) monochromator and Soller slits in front of the Pixcel detector.
  - θ/2θ scans to find orientation and phase presence in GaN core – oxide shell NWs.
  - 2θ/ω scans and reciprocal space maps (RSMs) of 0002, 0004, 0006 GaN symmetrical reflections and -1-124, -1015 GaN asymmetrical reflections.

  Analysis of XRD results:
  - simulation of symmetrical 2θ/ω scans by utilizing dynamical theory of X-ray diffraction.
  - calculation of lattice constants and strain relation from RSMs.

Raman spectroscopy:

- The micro-Raman measurements were performed at room temperature using the T64000 Horiba Jobin-Yvon spectrometer configured in a backscattering geometry.
- As a detector a liquid nitrogen cooled multichannel silicon CCD camera was used. A 532 nm semiconductor laser was used to excite the samples (non-resonant excitation).

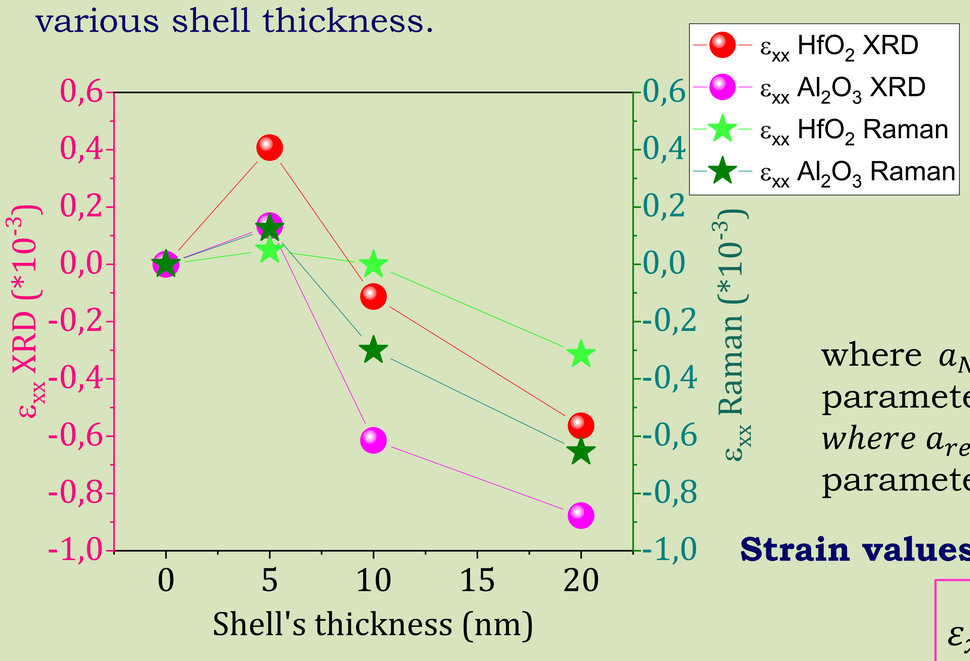
X-RAY DIFFRACTON RESULTS



XRD 2θ/ω scans of 0002 GaN reflection for GaN NWs with HfO_2 (a) and Al_2O_3 (b) shell of different thickness.

	Lattice constant c (Å)	Lattice constant a (Å)	XRD $\varepsilon_{zz} \cdot 10^{-3}$	XRD $\varepsilon_{xx} \cdot 10^{-3}$	Raman $\varepsilon_{xx} \cdot 10^{-3}$
Sample A-5	5.1808 Å	3.1953 Å	-0.81	0.14	0.13
Sample A-10	5.1807 Å	3.1929 Å	0.48	-0.61	-0.29
Sample A-20	5.1792 Å	3.1926 Å	0.52	-0.88	-0.65
Sample H-5	5.1834 Å	3.1924 Å	-0.23	0.41	0.05
Sample H-10	5.1801 Å	3.1941 Å	0.67	-0.11	-0.001
Sample H-20	5.1851 Å	3.1886 Å	0.35	-0.56	-0.31

The values of lattice constants obtained from XRD RSMs. The ε_{zz} and ε_{xx} strain component calculated from XRD and Raman measurements of GaN/oxide NWs of various shell thickness.



- strain values in in-plane direction from GaN-core part of NWs changes in the same way from Raman spectroscopy and XRD techniques,
- for the sample with the thinnest oxide shell the strain value change the sign.
- The thicker oxide shell the higher strain in in-plane and out-of-plane direction is observed.

Strain values from XRD:

$$\varepsilon_{xx} = \frac{a_{NW} - a_{relax}}{a_{relax}}$$

$$\varepsilon_{zz} = \frac{c_{NW} - c_{relax}}{c_{relax}}$$

where a_{NW}, c_{NW} - a and c lattice parameters of GaN core part of NW, *where* a_{relax}, c_{relax} - a and c lattice parameters of unstrained GaN NW.

Strain values from Raman spectroscopy:

$$\varepsilon_{xx} = \frac{\Delta\omega}{2\left(a - b\frac{c_{13}}{c_{33}}\right)}$$

where $\Delta\omega$ – is the difference between the position of the GaN-like E2 (high) Raman mode in the studied samples and pure GaN NWs,
a and b- phonon deformation potential parameters,
c_{13}, c_{33} - elastic constants of hexagonal GaN.

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