Strain distribution in GaN/AlN multi quantum wells studied by X-ray diffraction and photoluminescence

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Aim of the work:

- to apply X-ray diffraction (XRD) technique to study strain distribution in GaN/AlN multi-quantum-wells (MQWs) grown by plasma-assisted MBE on AlN/sapphire substrates
- to investigate an influence of well/barier thickness on strain state in MQWs

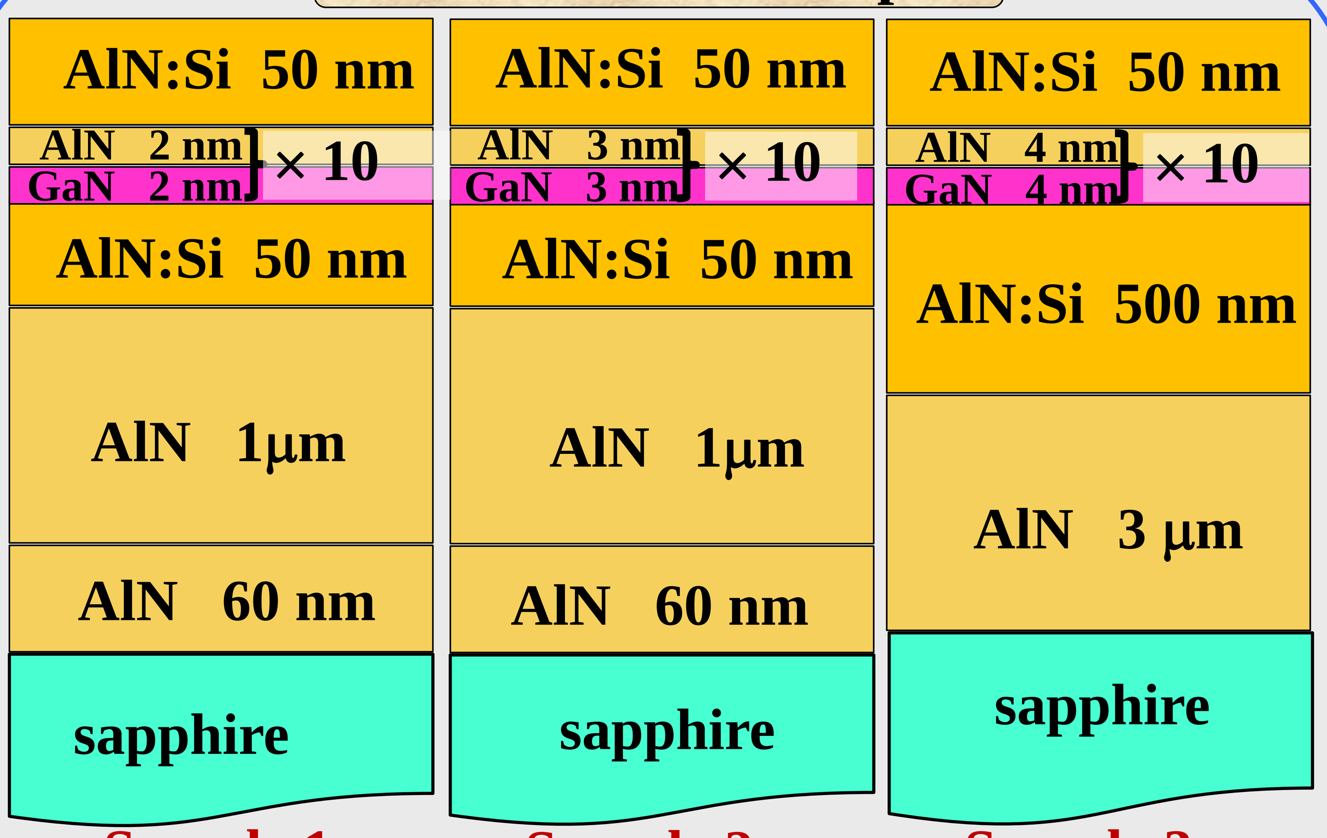
Samples studied:

- GaN/AlN MQWs with GaN well and AlN barrier thicknesses from 2nm to 4 nm
- structures grown on sapphire substrates with AlN layers by plasma assisted molecular beam epitaxy

Experimental techniques

- X-ray diffraction:
  - 2θ/ω scan of 00.2 AlN/GaN symmetrical reflection
  - reciprocal space map (RSM) of 11.4 AlN/GaN asymmetrical reflection
- Analysis of XRD results:
  - simulation of 00.2 symmetrical 2θ/ω scan by utilizing dynamical theory of X-ray diffraction
  - calculation of lattice constants and strain relation from RSMs
- Transmission electron microscopy (TEM):
  - to check the quality of MQWs interfaces and thicknesses of well/barrier
- Photoluminescence (PL):
  - to compare spectrum coming from MQWs in dependence of well/barrier thickness

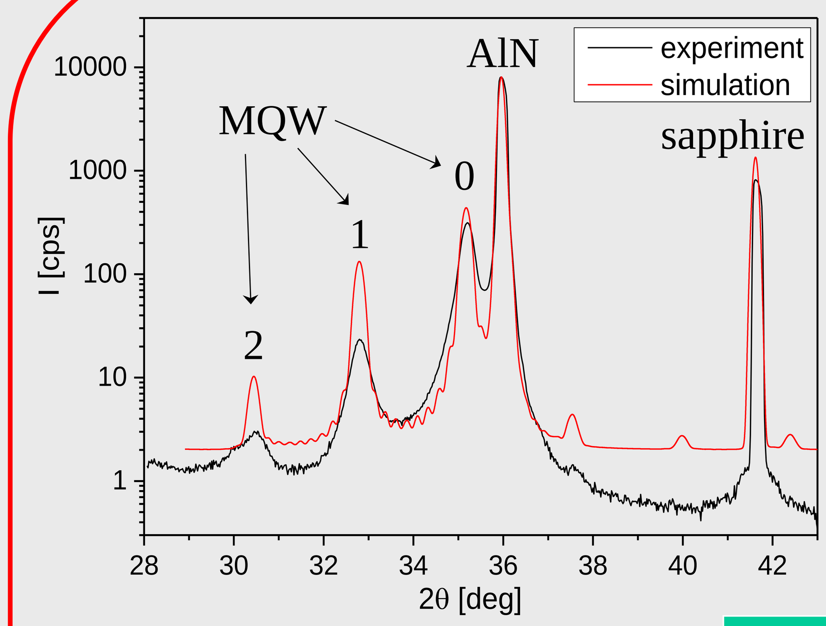
Structure of the samples

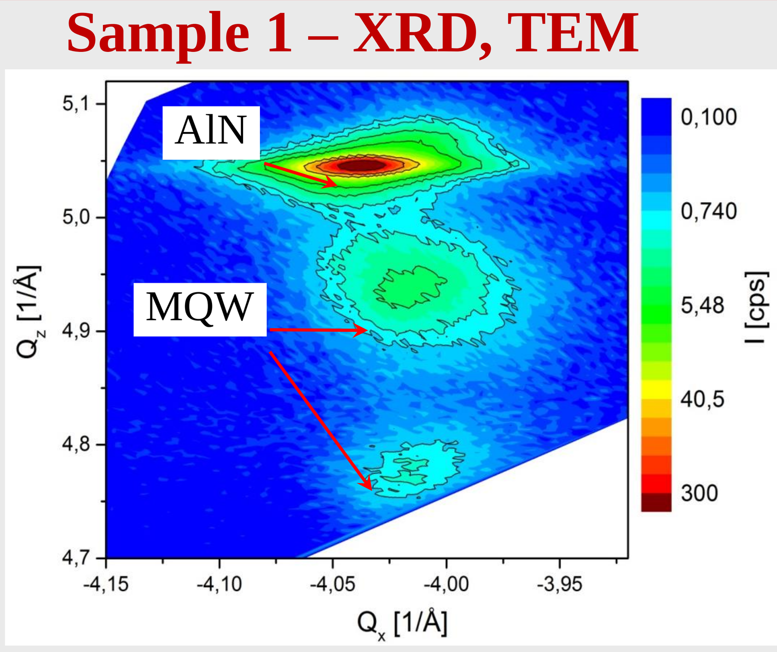


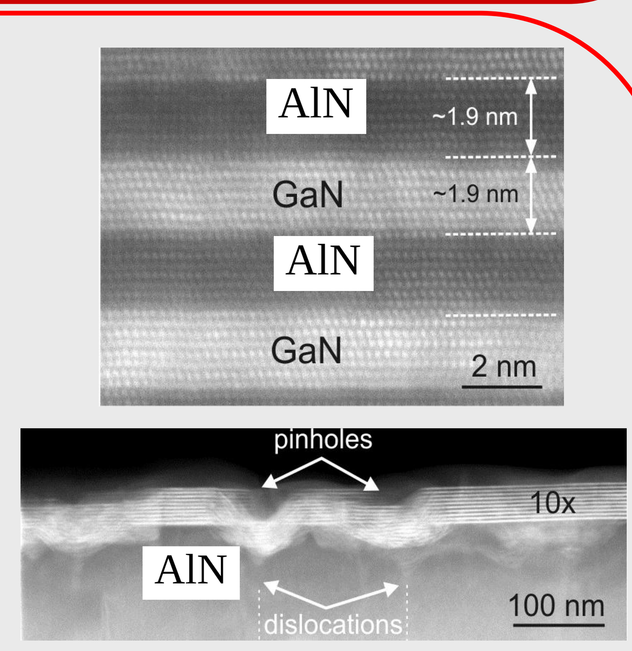
Sample 1 Sample 2 Sample 3

Theoretical values of lattice constants:
c_{MQW}=5.0834Å; a_{MQW}=3.1512 Å
It corresponds to composition of $Al_xGa_{1-x}N$ **with x=0.5**

Sample 1 – XRD, TEM





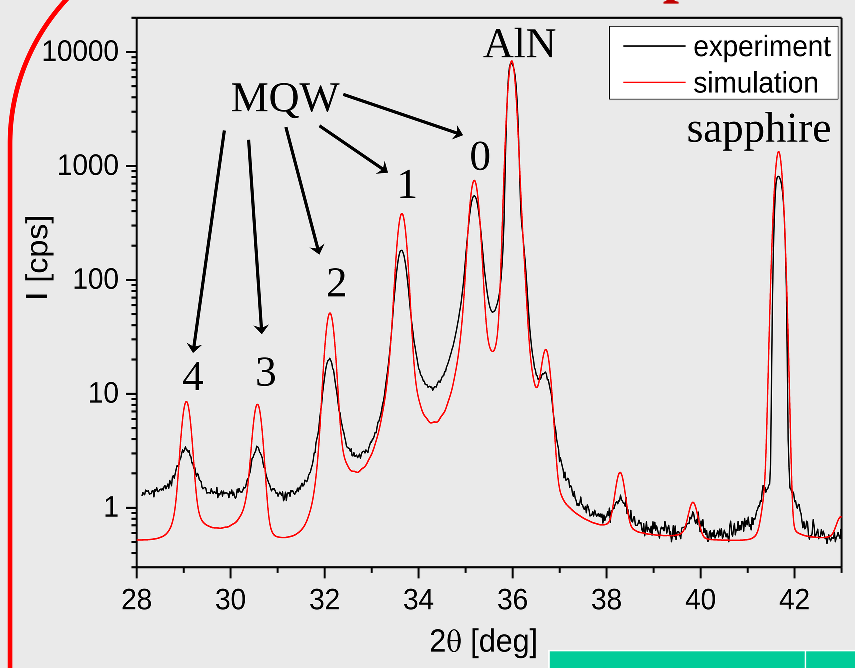


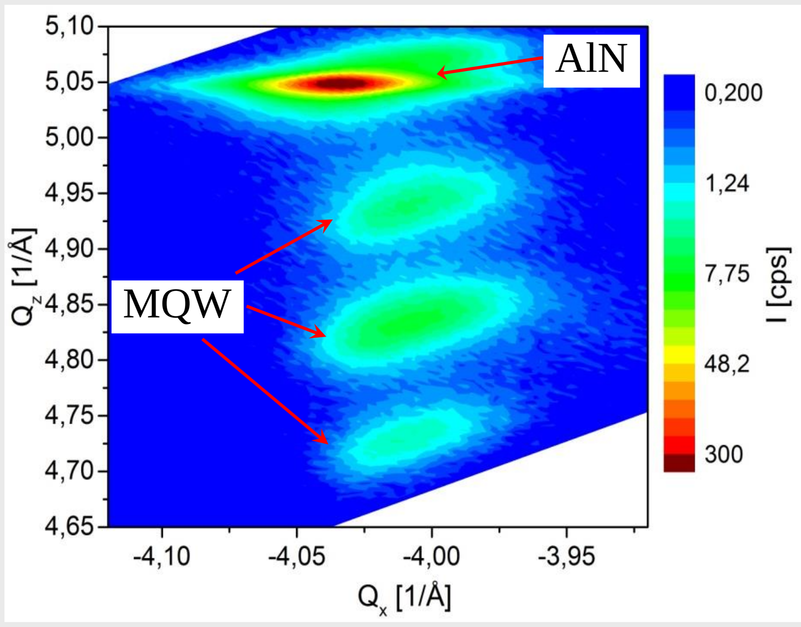
- Experimental 2θ/ω scan of AlN/GaN 00.2 reflection shows 2nd order of peaks coming from MQWs
- Theoretical curve of 2θ/ω scan of AlN/GaN 00.2 reflection is in a good agreement with experimental data
- The intensities varied because of the interface blurring and pinholes existing in the structure

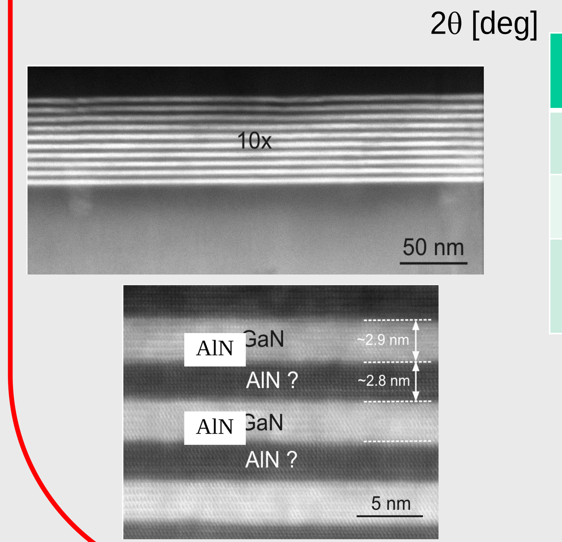
Simulation	Thickness (nm)	Lattice constants
AlN	1.93	c_{MQW} = 5.0957 Å a_{MQW} = 3.1209 Å (it corresponds to composition of $Al_xGa_{1-x}N$ **with x=0.56**)
GaN	1.95	
Total MQW	38.8	

- TEM images show good quality of interfaces in MQWs
- There are pinholes present in the structure
- RSM of 11.4 assymetrical reflection shows partial relaxation of AlN/GaN MQWs
- Relaxation is equal to 30%

Sample 2 – XRD, TEM



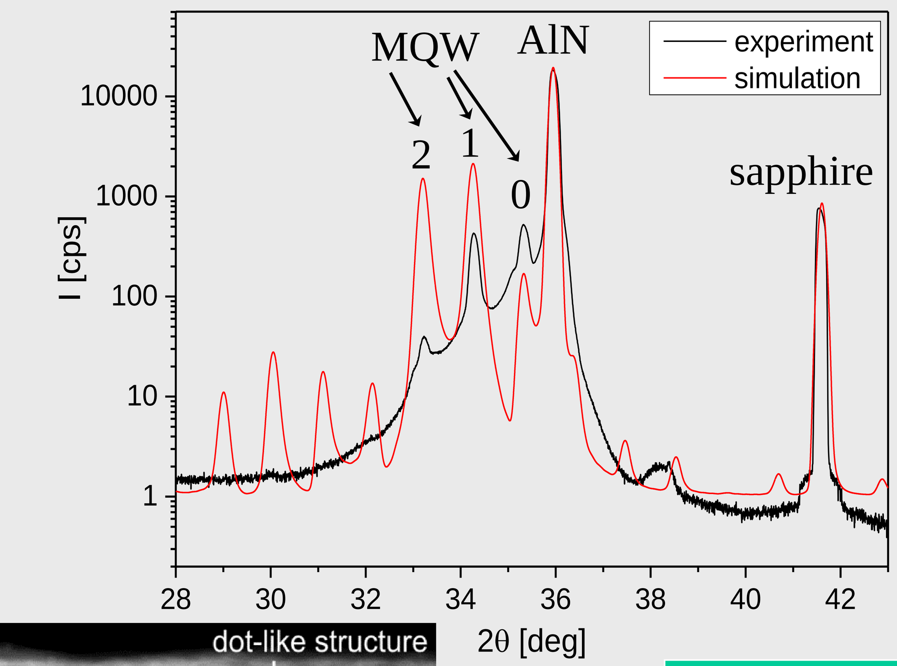


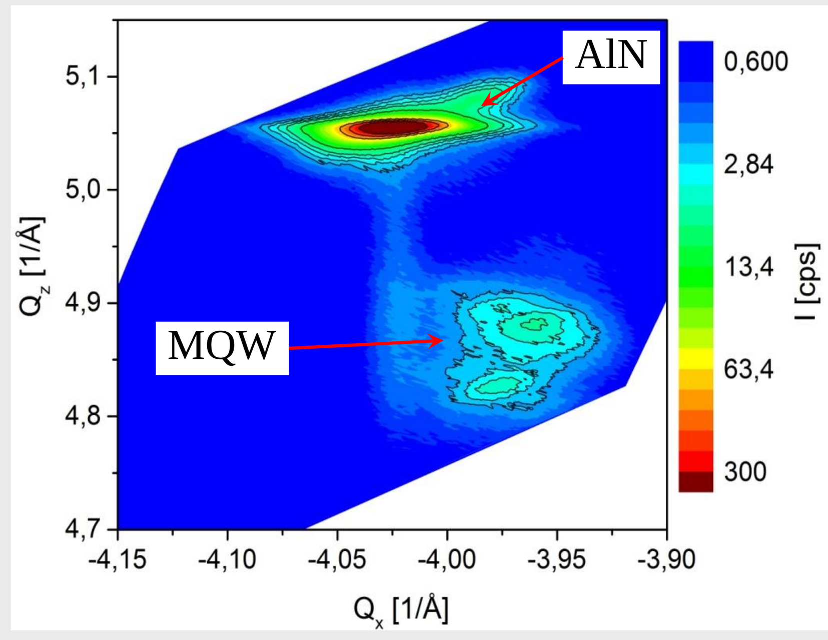


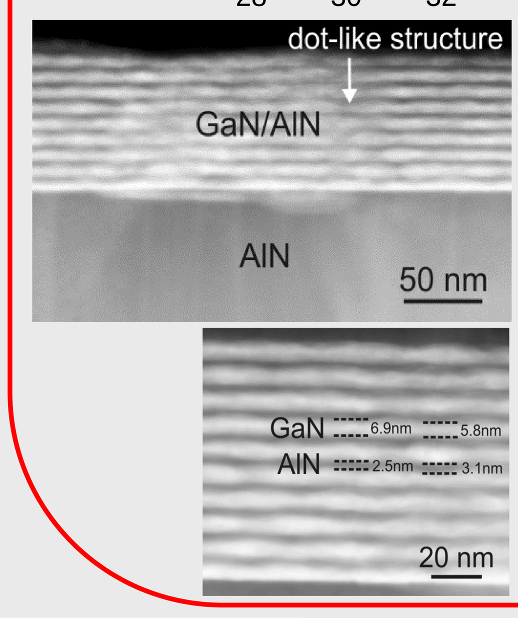
Simulation	Thickness (nm)	Lattice constants
AlN	3	c_{MQW} = 5.0950 Å a_{MQW} = 3.1275 Å (it corresponds to composition of $Al_xGa_{1-x}N$ **with x=0.54**)
GaN	3	
Total MQW	60	

- Experimental 2θ/ω scan of AlN/GaN 00.2 reflection shows 4th order of peaks coming from MQWs
- RSM of 11.4 assymetrical reflection shows partial relaxation of AlN/GaN MQWs (relaxation = 27%)
- Very good quality of MQWs from TEM

Sample 3 – XRD, TEM



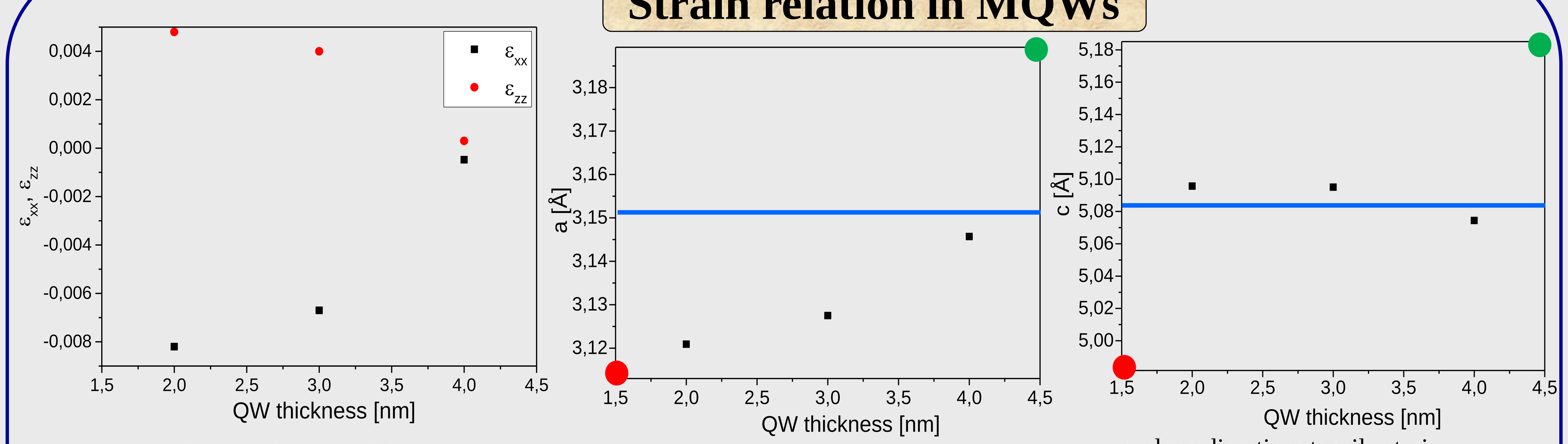




Simulation	Thickness(nm)	Lattice constants
AlN	2.3	c_{MQW} = 5.0744 Å a_{MQW} = 3.1457 Å (it corresponds to composition of $Al_xGa_{1-x}N$ **with x=0.55**)
GaN	6.3	
Total MQW	86	

- Experimental 2θ/ω scan of AlN/GaN 00.2 reflection shows only 2nd order of peaks coming from MQWs
- RSM of 11.4 assymetrical reflection shows partial relaxation of AlN/GaN MQWs (relaxation = 30%)
- Bad quality of MQWs from TEM; pinholes, dot-like structure

Strain relation in MQWs



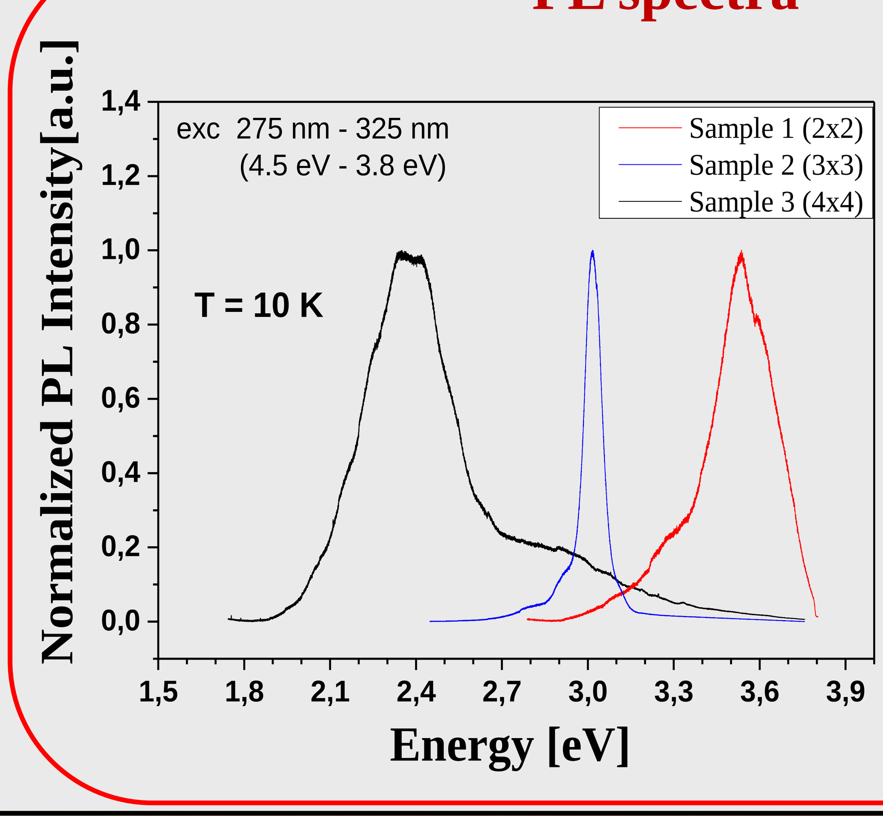
- Strain values calculated from experimental and relaxed lattice constants
- Thicker MQW trend to relaxed state

$Al_{0.5}Ga_{0.5}N$: a = 3.1512Å, c = 5.0834Å
GaN: a = 3.1893Å, c = 5.1851Å
AlN: a = 3.1130Å, c = 4.9816Å

a-plane direction: tensile strain

c-plane direction: compressive strain

PL spectra



- PL spectra reveal red-shift of the **peak energies** even below the PL peak energy of bulk GaN (3.48 eV) with increasing QW width; this is connected with Quantum Confined Stark Effect (QCSE)
- Sample 2 has the best quality (the peak is narrow)
- For Sample 1 and 3 we observe some **multipeak structure** of PL spectra which can be connected with the strong thickness fluctuations in MQWs
- The broadening of peaks can be caused by the inhomogenities of the samples and interfaces smoothness

Conclusions

- For Sample 1 and 3 we observe existence of the pinholes or dot-like structure which lead to worse quality of XRD peaks; only few peaks coming from MQW are registered
- Sample 2 has the best quality, it has smooth interfaces; there are visible 4th order XRD peaks coming from MQWs
- MQWs with well and barrier thicknesses from 2 nm to 4 nm are in tensile strain in in-plane direction and in compressive strain in out-of-plane direction
- The thicker well/barrier is the more relaxed MQWs are
- Luminescence properties of the samples correlate well with XRD and TEM results: the better sample quality, the more efficient luminescence and narrow PL peak
- The PL spectra show red-shift with increasing of well/barrier thickness, which is connected with QCSE