STREEM: STRain Engineering in Electronic Materials

AlGaN Edition

2023

(0001) III-Nitrides

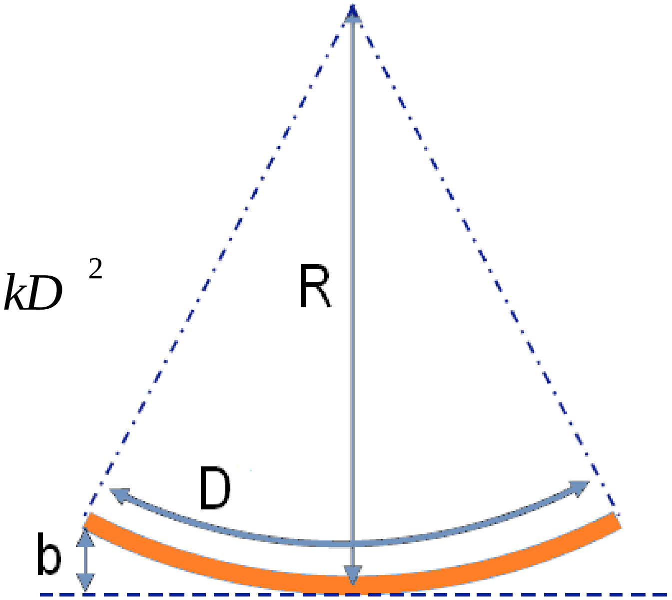
STREEM-AlGaN may be used to analyze:

- Evolution of curvature at the stages of heating, growth, and cooling of the structure under various process parameters and sequences of the layers;
- Stress relaxation in compressively stressed layers and dislocation dynamics;
- Crack formation induced by tensile stress both during the growth and after cooling of the structure;
- Influence of the process parameters on the through-wafer temperature drop and its contribution to the structure bow
- Stress state in the particular layers via processing of in-situ curvature data

Curvature and bow: basic definitions

- Curvature radius R, wafer diameter D
- Curvature k: $k = \frac{1}{R}$
- Wafer bow *b:* $b(k, D) = R\left(1 - \cos\frac{D}{2R}\right) \approx \frac{1}{8} k D^2$
- Wafer bow is proportional to curvature and

square of wafer diameter



k>0 ↔ tensile stress (positive) ↔ concave bowing ↔ 

k<0 ↔ compressive stress (negative) ↔ convex bowing ↔ 

Growth stage:

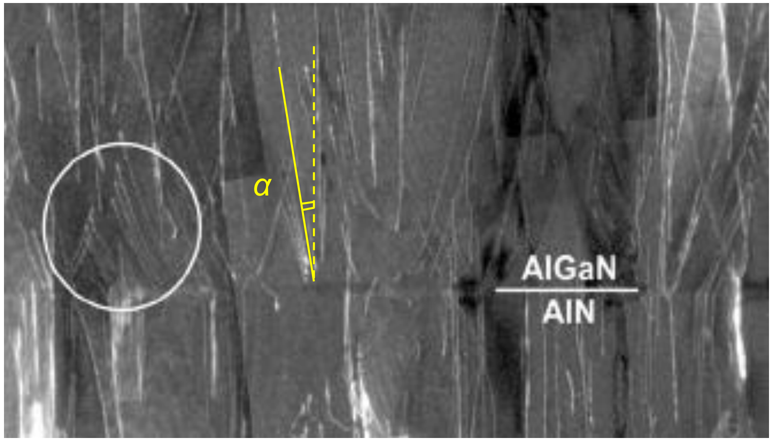
stress, curvature, and dislocation dynamics

Compressive stress relaxation

Inclination of a-type threading dislocations (TDs)

⇩

Annihilation of TDs (reduction of TD density)

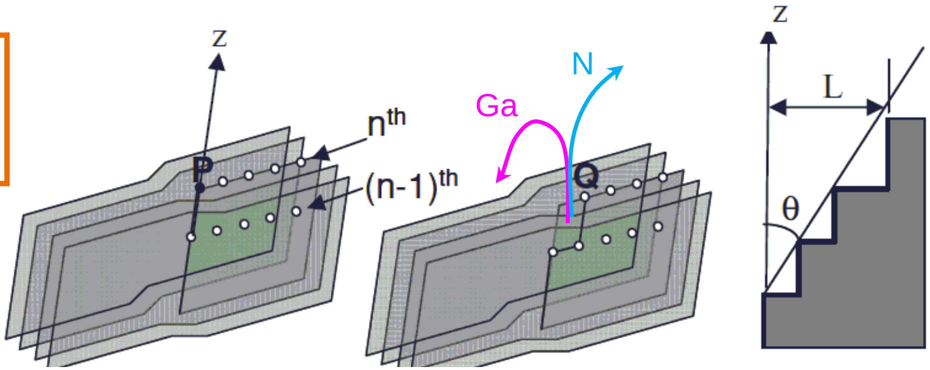


D.M. Follstaedt et al., J. Appl. Phys. 83 (2003) 2569

Inclination of TDs is modeled as core-atoms outdiffusion

⇩

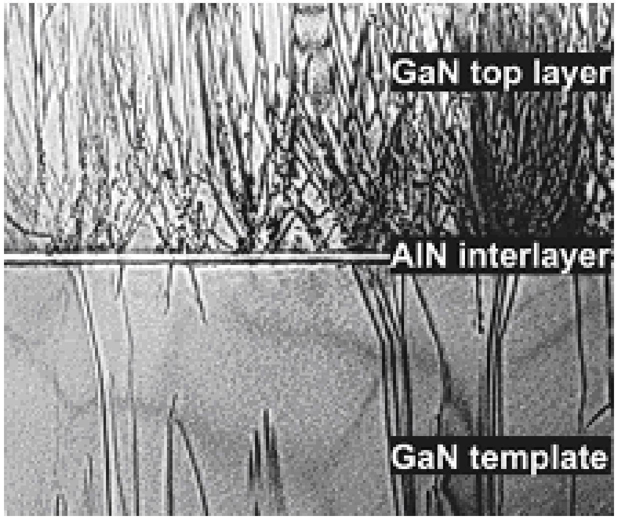
$$\alpha = \alpha\,(T\,,\,G_R,\,\sigma_{surf}\,,\,[Si]\,,\,\rho_{TD})$$



S. Raghavan, Phys. Rev. 83 (2011) 052102 ;
S. Raghavan et al., Cryst. Growth 359 (2012) 35

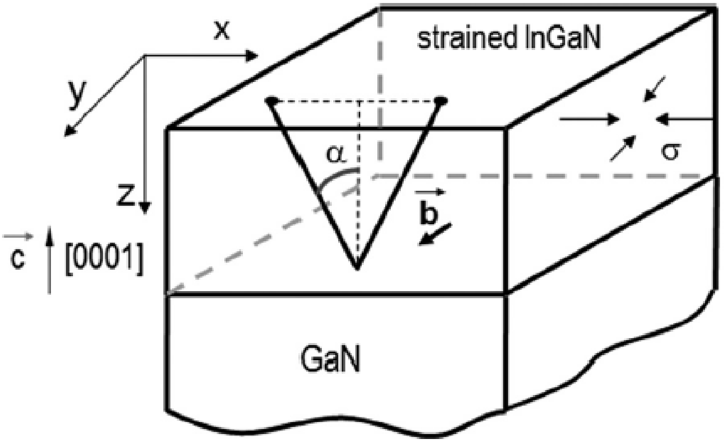
Nucleation of new TDs in GaN layers

Nucleation of new TDs in highly compressively strained GaN layers



J.F. Wang, Appl. Phys. Lett. 89 (2006) 152105

Generation of new dislocations is predicted, when the work of compressive stress exceeds the elastic energy associated with the dislocations

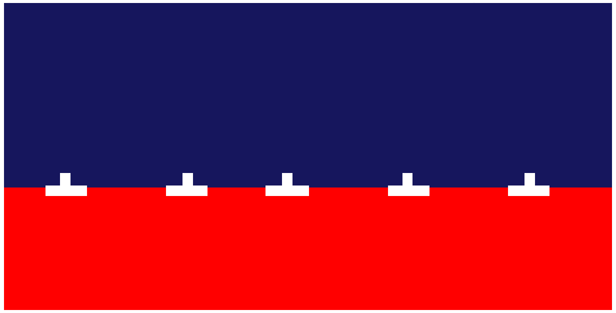


A.V. Lobanova et al., Appl. Phys. Lett. 103 (2013) 152106

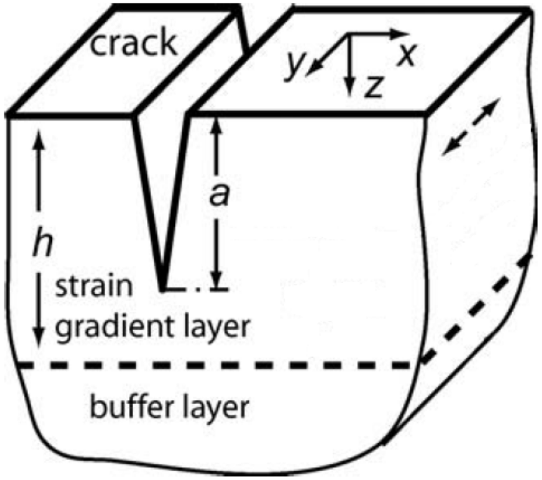
Tensile stress relaxation. AlGaN interlayers

Al(Ga)N layers are normally tensely strained ⇨ Different relaxation mechanisms

Generation of in-plane misfit dislocations (at low thickness)



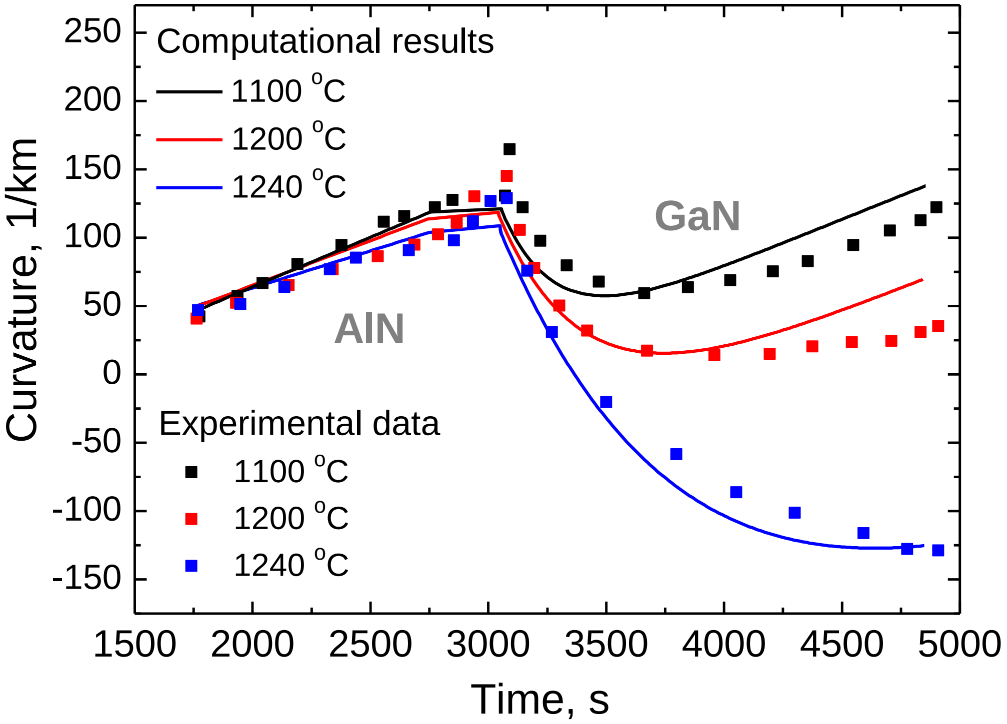
Cracking of the layer



Curvature vs dislocation density in GaN/AlN structure

AlN has higher dislocation density at lower growth temperatures.

Higher dislocation density in GaN (inherited from AlN) results in faster stress relaxation due to inclination of the dislocations.



ρ_{TD}~$6.0 \cdot 10^{10}$

ρ_{TD}~$3.8 \cdot 10^{10}$

ρ_{TD}~$1.8 \cdot 10^{10}$

Wafer: Si, 50 mm

Purpose: high quality AlN for GaN/Si growth

Structure: (115nm) AlN / (1.7µm) GaN

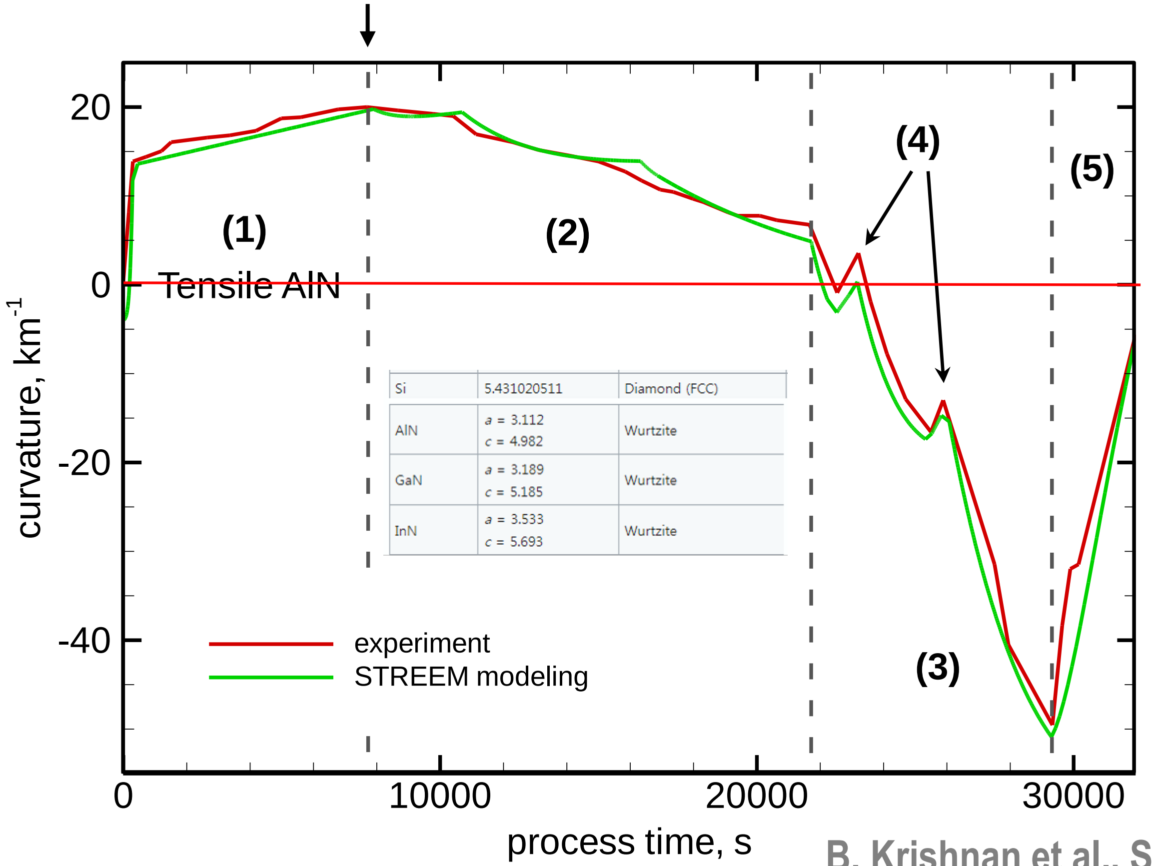
C. Liu et al., Phys. Stat. Sol. C 10, 11 (2013) 1541

Use of AlGaN graded buffers for strain engineering

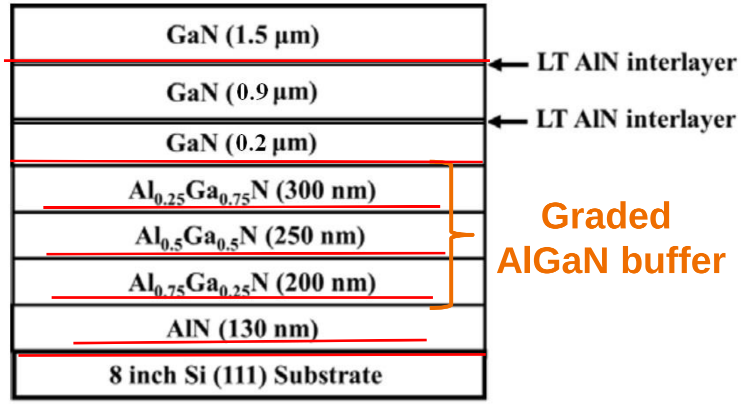
Wafer: Si, 200 mm

Purpose: GaN/Si buffer with flat surface

TDD was specified here



Si	5.431020511	Diamond (FCC)
AlN	a = 3.112 c = 4.982	Wurtzite
GaN	a = 3.189 c = 5.185	Wurtzite
InN	a = 3.533 c = 5.693	Wurtzite

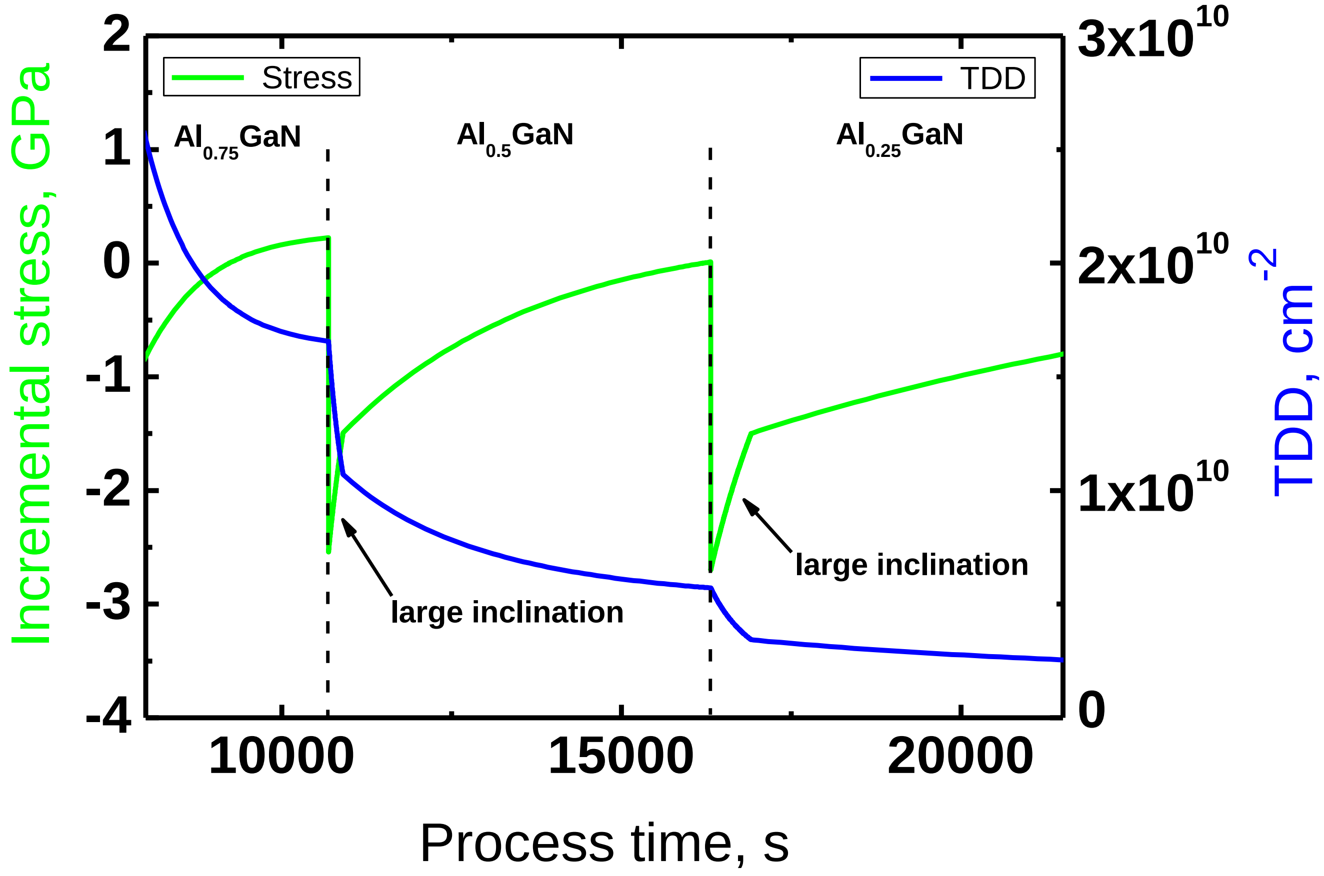


STREEM predicts well the curvature measured @RT

(1): AlN nucleation
(2): AlGaN graded buffer
(3): thick GaN
(4): AlN interlayers
(5): cooling

B. Krishnan et al., Sensors and Materials 25 3 (2013) 205

Use of AlGaN graded buffers for strain engineering (Continued). Evolution of stress and dislocations



Closer look at the graded AlGaN buffer shown also in segment (2) of the plot on the previous page

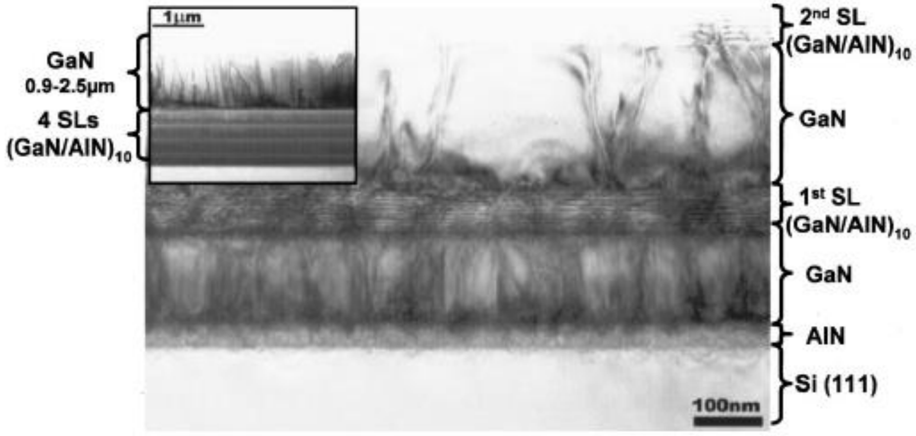
Gradual decrease of the dislocation density, ultimately, by an order of magnitude, in the graded AlGaN buffer.

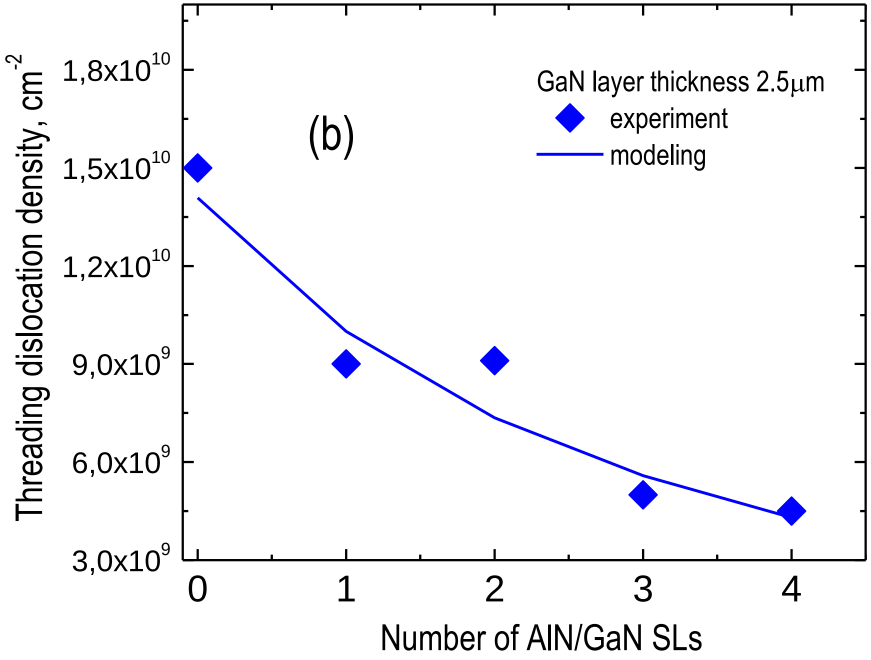
Large inclination of the threading dislocation due to high mismatch stress

B. Krishnan et al., Sensors and Materials 25, 3 (2013) 205

GaN/AlN SL as alternative buffer structure: experimental facts

Wafer: Si
Purpose: crack free thick GaN-on-Si
Buffer structure: 4x(GaN/AlN SL) separated by 200 nm GaN

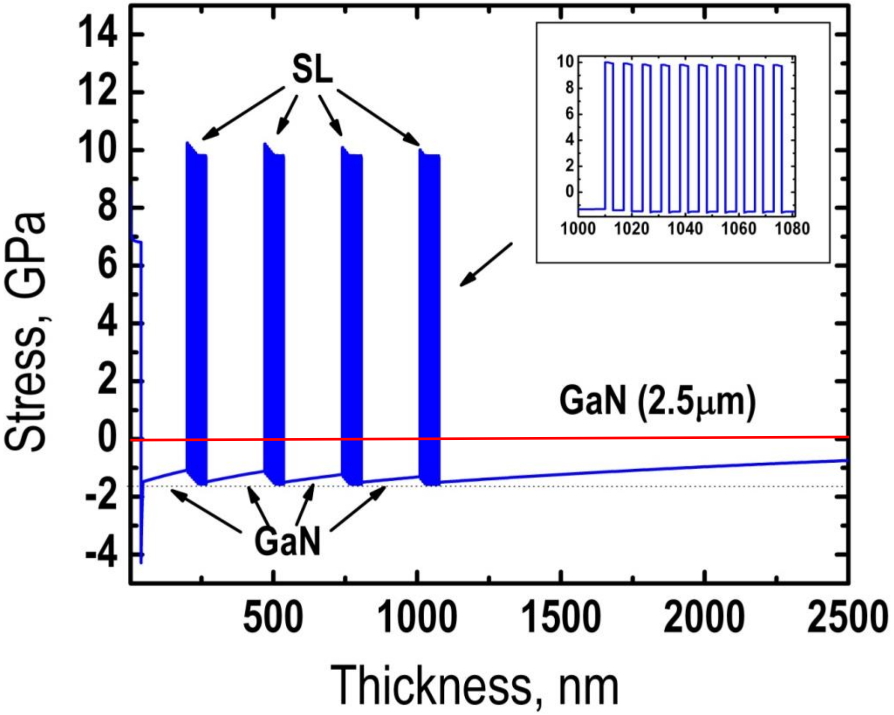


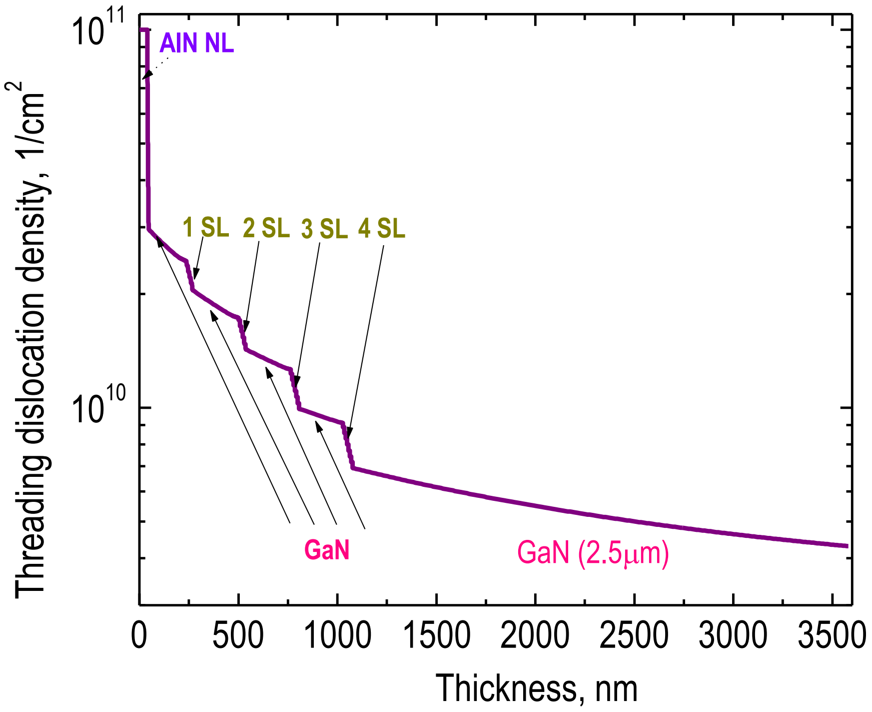


- ✓ Superlattices can efficiently counteract the tensile stress usually observed in GaN on Si
- ✓ Reduction of the dislocation density with the number of SLs
- ✓ Crack-free 2.5 µm thick GaN can be grown on this buffer structure

E. Feltin et al., Appl. Phys. Lett. 79 (2001) 3230

GaN/AlN SL as alternative buffer structure: modeled stress and TDD evolution



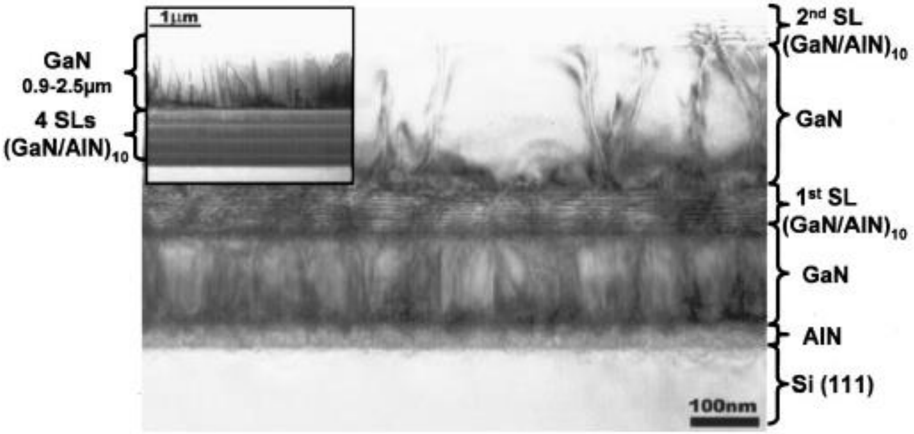


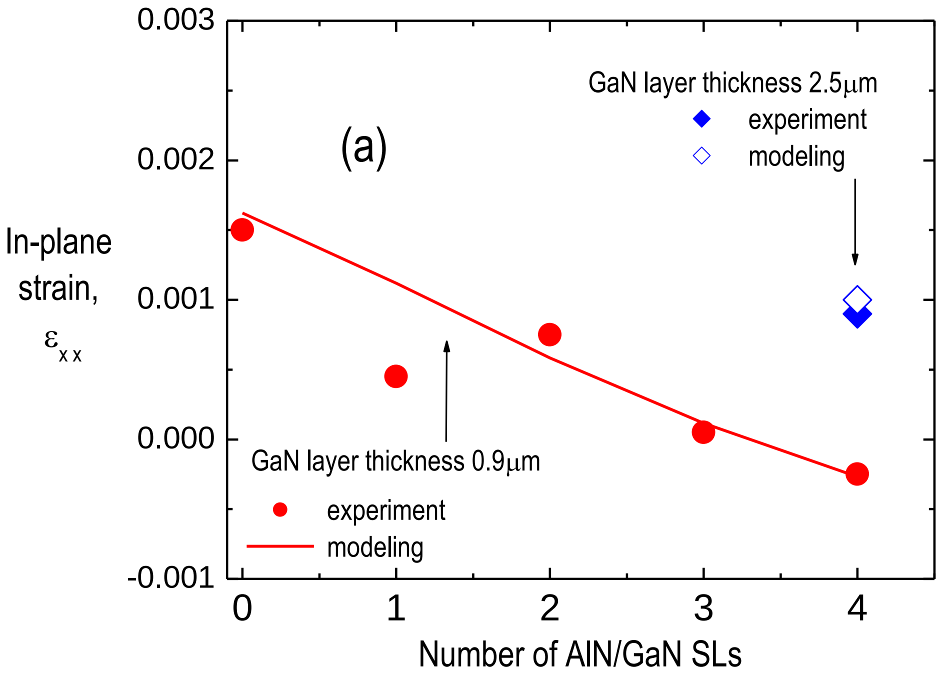
- high stress in the first GaN layer results in nucleation of new dislocations and fast reduction of their density due to large inclination and annihilation.
- thin AlN layers in the SLSs are far from being fully relaxed.
- formation of new dislocations in GaN layers is not predicted. Instead, the dislocation density decreases gradually throughout the supperlattices and in the GaN layers in-between

E. Feltin et al., Appl. Phys. Lett. 79 (2001) 3230

Stress state in the structure with GaN/AlN SLs

Wafer: Si
Purpose: crack free thick GaN-on-Si
Buffer structure: 4x(GaN/AlN SL) separated by 200 nm GaN

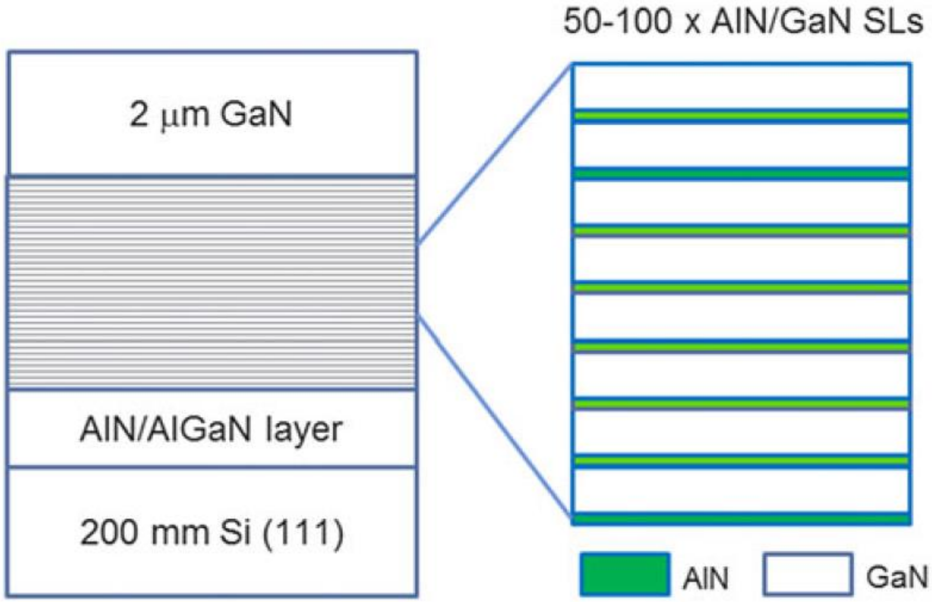




About linear decrease of the in-plane strain of the GaN layers with the number of superlattices used in the structure is reproduced well by the modeling

E. Feltin et al., Appl. Phys. Lett. 79 (2001) 3230

AlN/GaN SL structures



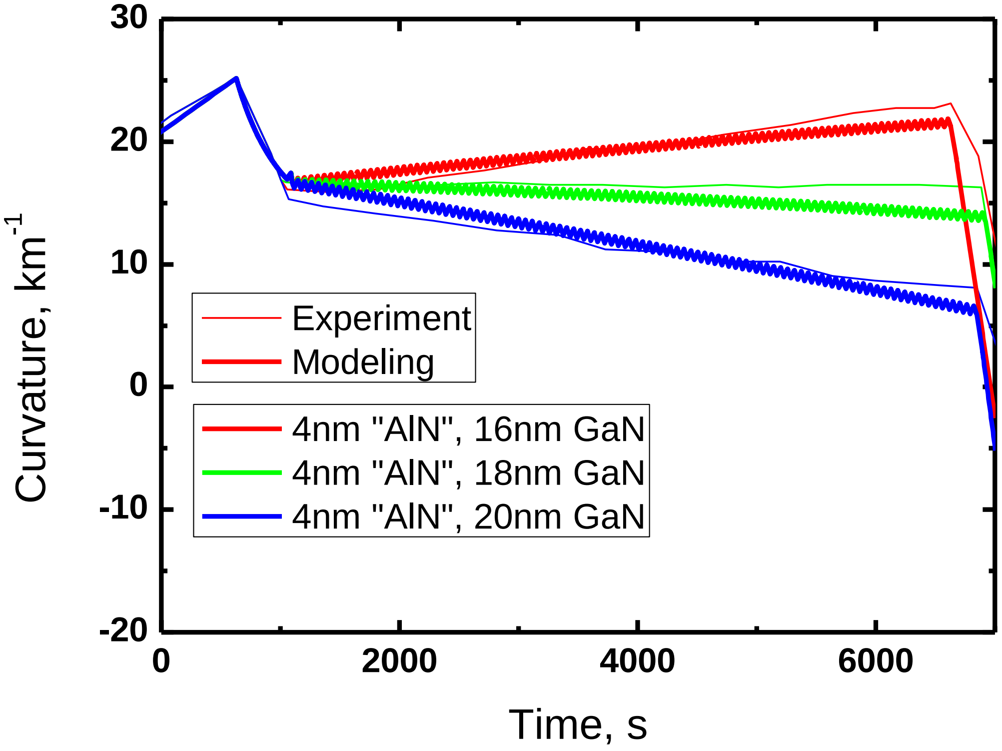
- ✓ 1 mm thick 200 mm Si wafer
- ✓ Structure includes:
  - 100 nm AlN nucleation layer
  - 100 nm $Al_{0.24}GaN$ intermediate layer
  - 50-100 period AlN/GaN SL
  - 1-2 µm GaN thick layer

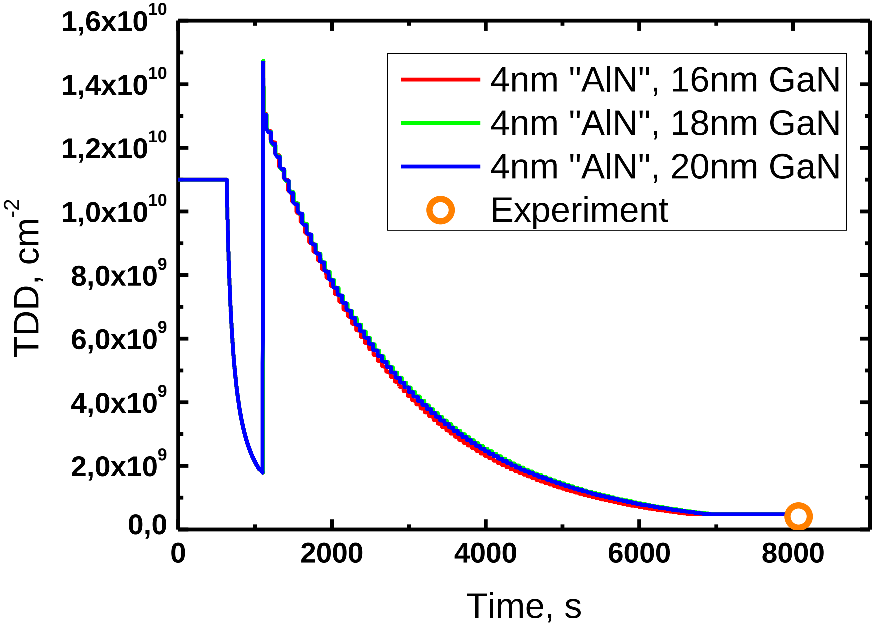
Two series of experiments:

1. GaN thickness in the SL is varied (16-18-20 nm) with constant AlN thickness (4 nm)
2. AlN thickness in the SL is varied (2.5-3.5-4.5 nm) with constant GaN thickness (18 nm)

G.D. Papasouliotis et al., ECS Transactions 69 (11) (2015) 73
J. Su et al., J. Mater. Res. 30 (19) (2015) 2846
J. Su et al., Mater. Res. Soc. Symp. Proc. 1736 (2014) doi:10.1557/opl.2014.942

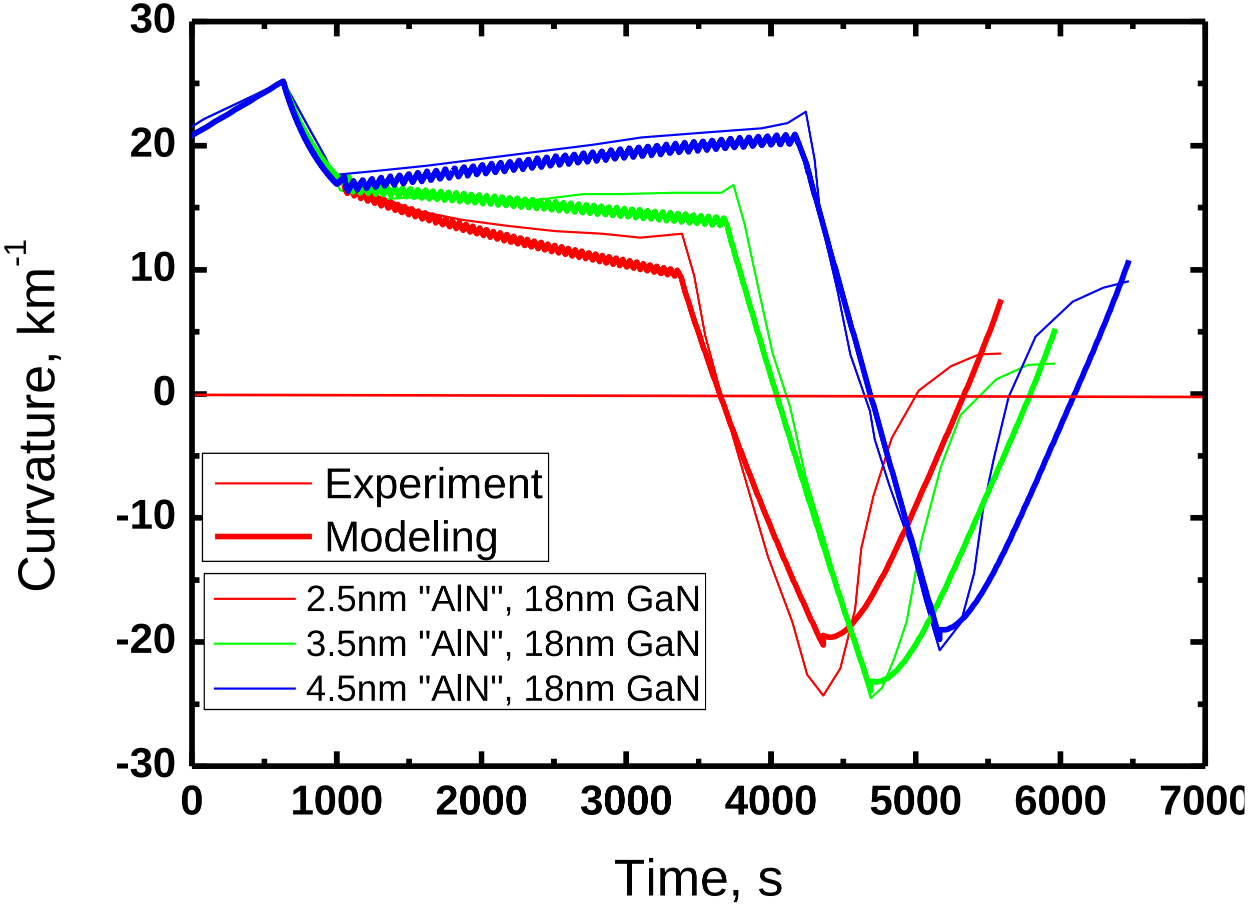
100x AlN/GaN SL with variable GaN period thickness



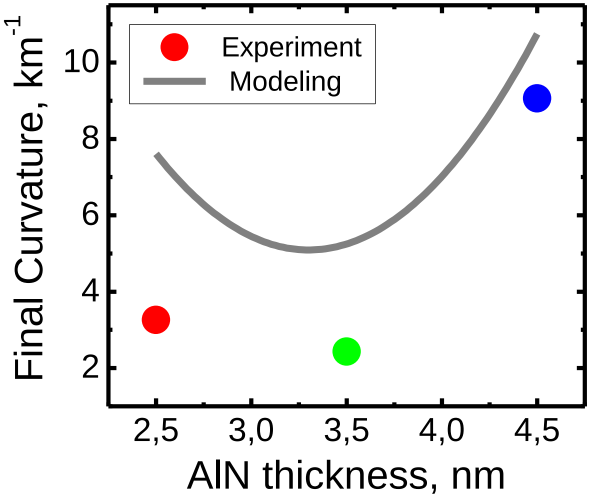


- **Increase of GaN period thickness enhances the compressive stress build-up in SL;**
- **New TDs are generated at first GaN period of SL**
- **GaN thickness variation has no effect on TDD evolution**

50x AlN/GaN SL with variable AlN thickness

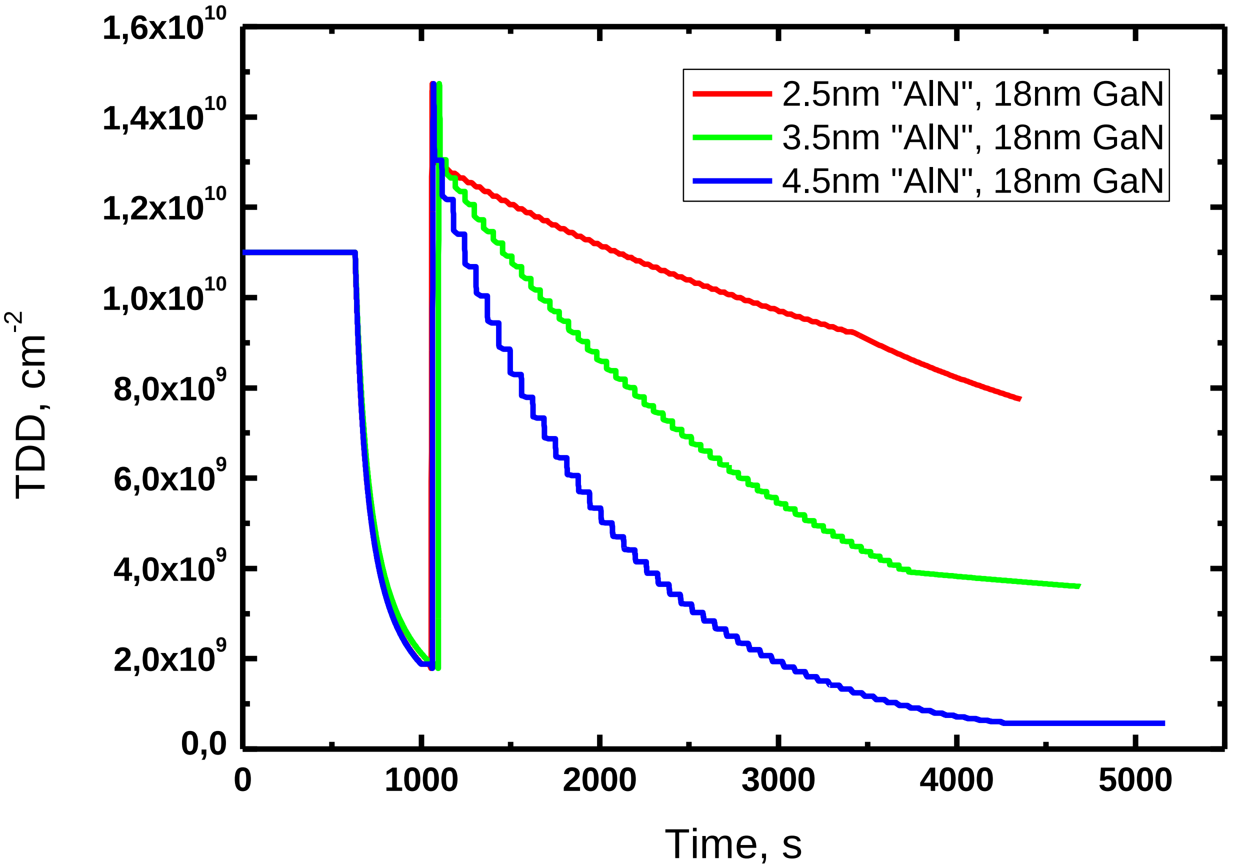


- ✓ 50x AlN/GaN SL
- ✓ 1 µm upper GaN
- ✓ Constant GaN thickness
- ✓ Variable AlN thickness



- Decrease of the AlN period thickness enhances the compressive stress build-up in the superlattice
- RT curvature dependence on AlN thickness is nonmonotonic

50x AlN/GaN SL with variable AlN thickness

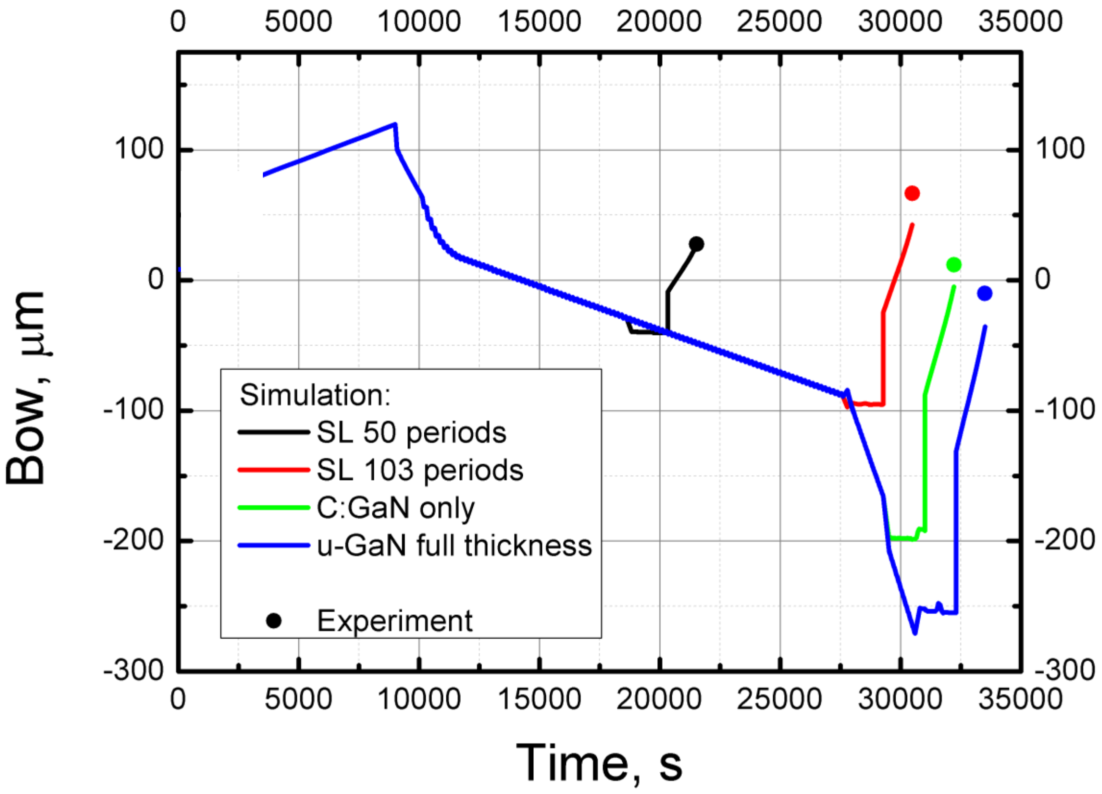


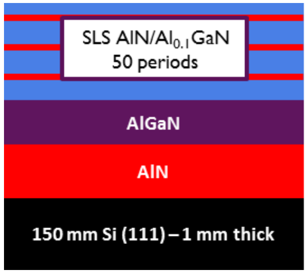
- ✓ 50x AlN/GaN SL
- ✓ 1 µm upper GaN
- ✓ Constant GaN thickness
- ✓ Variable AlN thickness

- Increase of the AlN thickness results in lowering of the final dislocation density
- SLs with the lowest AlN thickness is not so effective due to insufficient AlN relaxation

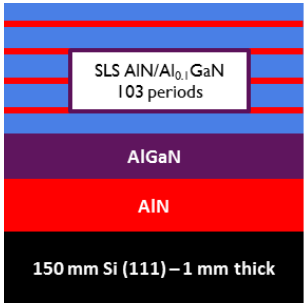
Stop-growth experiments

M. Rudinsky et al., Jpn. J. Appl. Phys. 58, SCCD26 (2019)

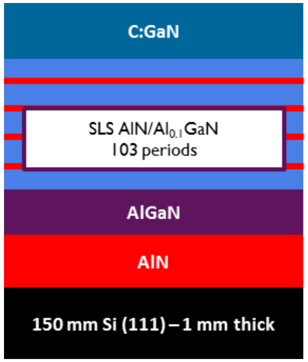




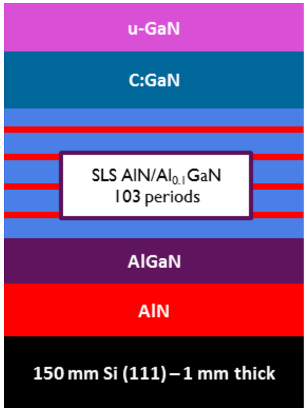
SL 50 periods



SL 103 periods



C:GaN only



u-GaN full thickness

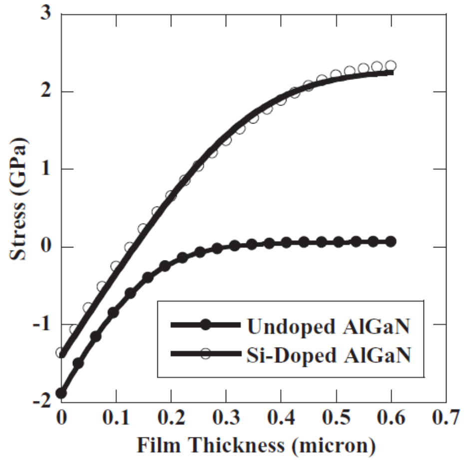
Stop-growth experiments to evaluate the impact of individual buffer parts on RT bow

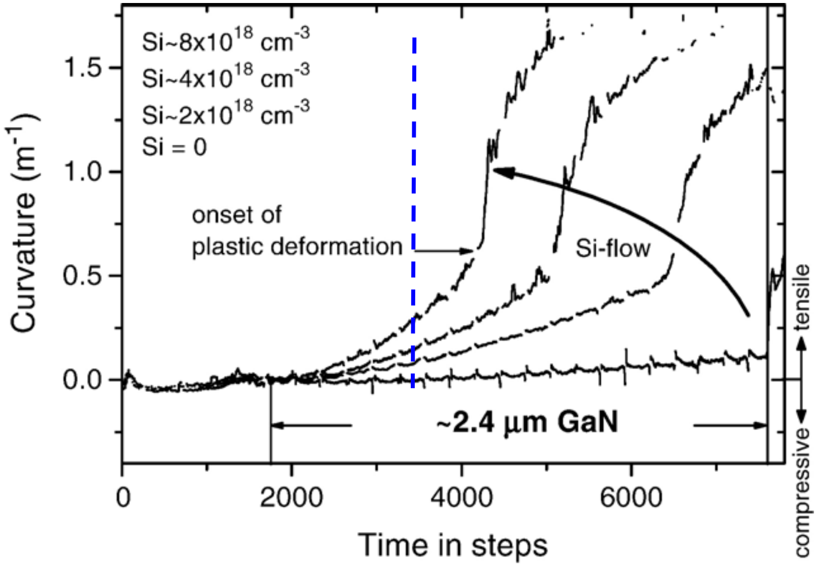
- **RT bow is predicted for various thickness and composition of the stack**
- **Plastic relaxation in silicon wafer is not expected**

Effect of Si doping on stress evolution

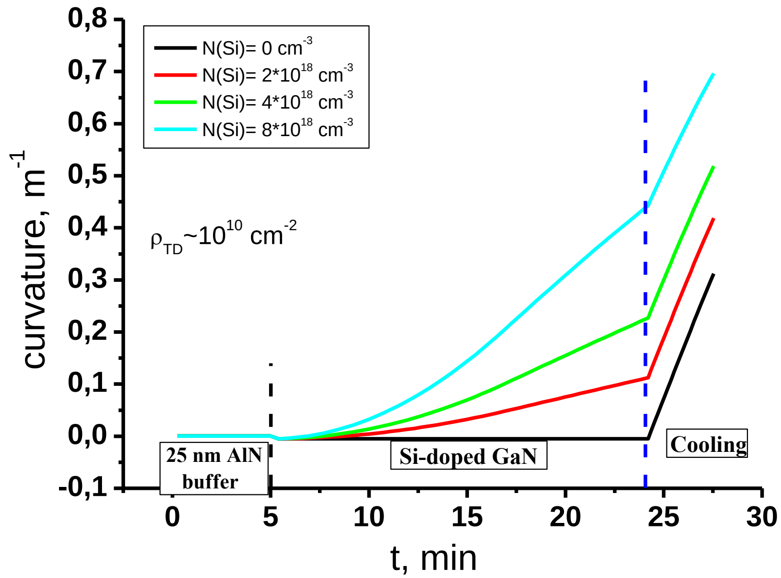
Modeling approach

- Si doping of (Al)GaN layers leads to enhancement of TDs inclination and increase of the tensile stress value at which TDs inclination ceases;
- Si doping accelerates relaxation of compressive stress and increases annihilation of TDs;
- The generated tensile stress persists even if Si-doping is stopped, since no mechanism exists which inverts the dislocation inclination;





275µm, 2 inch Si(111) wafer



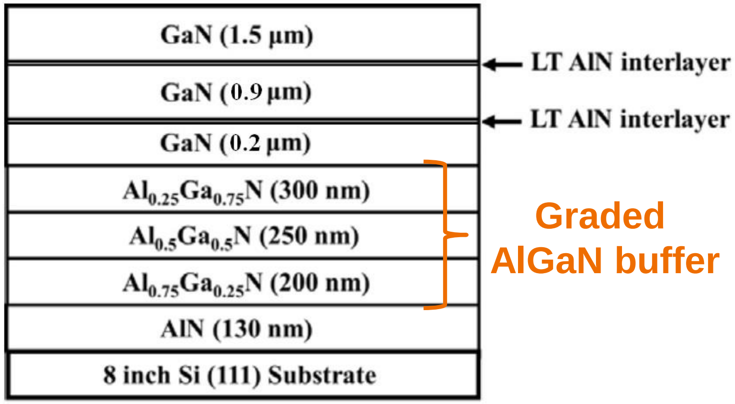
Modeling reproduces fairly well the experimental trends with respect to the curvature vs the doping level

Structure cooling:

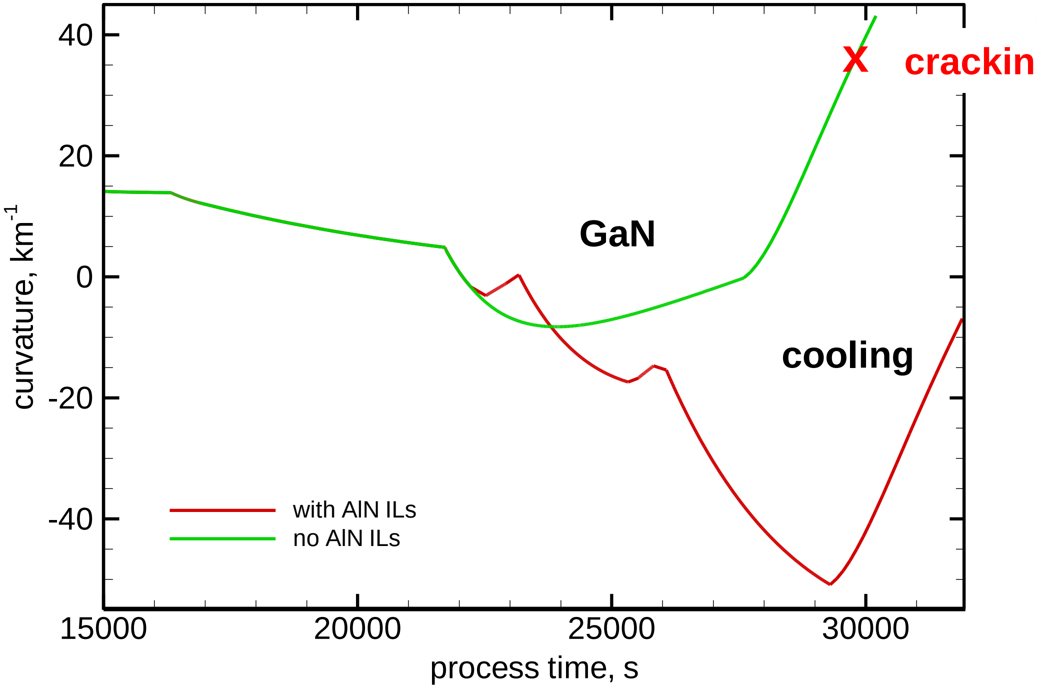
stress, bow, cracking

Insertion of AlN ILs at the stage of thick GaN growth

Wafer: Si, 200 mm
Purpose: GaN/Si buffer with flat surface


GaN (1.5 µm)
LT AlN interlayer
GaN (0.9 µm)
LT AlN interlayer
GaN (0.2 µm)
$Al_{0.25}Ga_{0.75}N$ (300 nm)
$Al_{0.5}Ga_{0.5}N$ (250 nm)
$Al_{0.75}Ga_{0.25}N$ (200 nm)
AlN (130 nm)
8 inch Si (111) Substrate

Graded AlGaN buffer



When AlN interlayers do not introduce additional compressive stress into the structure, cracked structure is predicted after cooling

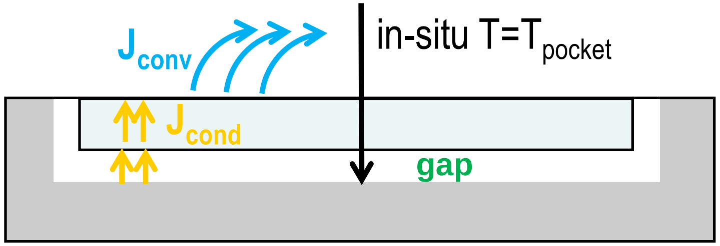
B. Krishnan et al., Sensors and Materials 25, 3 (2013) 205

Temperature drop:

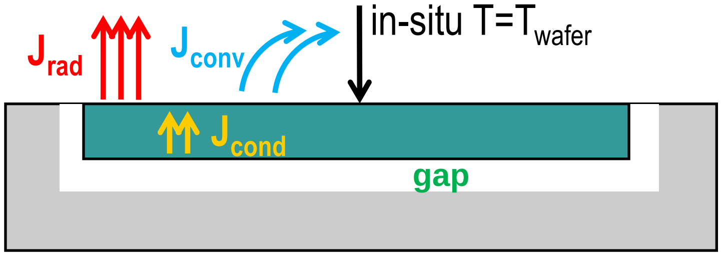
Bottom-to-top temperature gradient over substrate thickness

Temperature drop across the wafer

1D approach: temperature drop ΔT is estimated from known in-situ temperature via balance of heat fluxes (conductive J_{cond}, radiative J_{rad}, convective J_{conv}) through pocket-to-wafer gap, wafer, and reactor



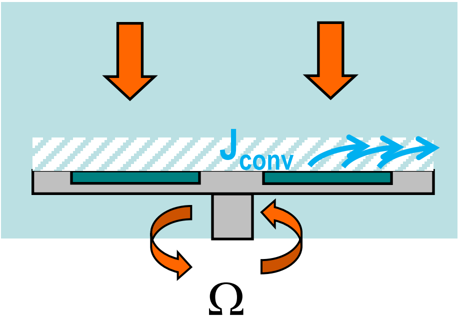
1) Sapphire wafer (*transparent*)



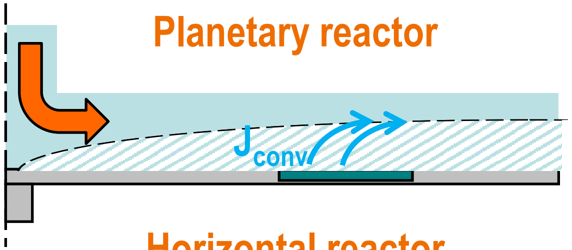
2) Silicon wafer (*opaque*)

For each reactor type, specific model allows to estimate contribution of convective heat exchange for a given set of process parameters

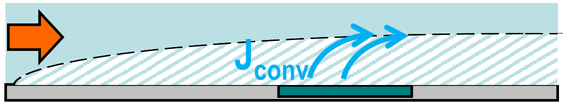
Rotating Disk Reactor



Planetary reactor



Horizontal reactor



Close coupled showerhead reactor