STREEM: STRain Engineering in Electronic Materials

AlGaN Edition

2016
STR Group

Overview of applications

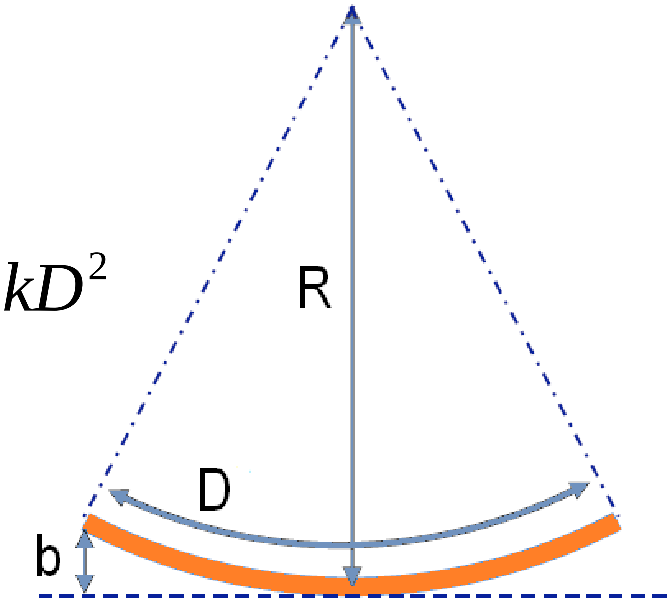
STREEM-AlGaN may be used to analyze:

- 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 tress 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: $k = \dfrac{1}{R}$
- Wafer bow *b:* $b(k,D) = R\left(1 - \cos\dfrac{D}{2R}\right) \approx \dfrac{1}{8}kD^2$
- Wafer bow is proportional to curvature and

square of wafer diameter



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

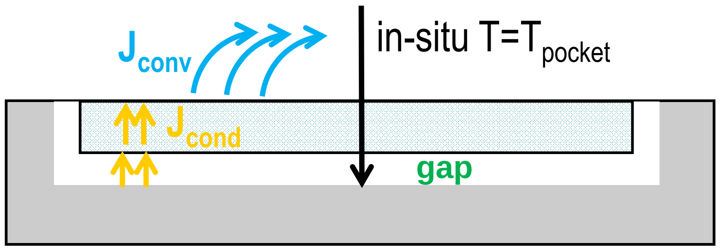
k<0 ↔ compressive stress (negative) ↔ convex bowing ↔

Heating stage:

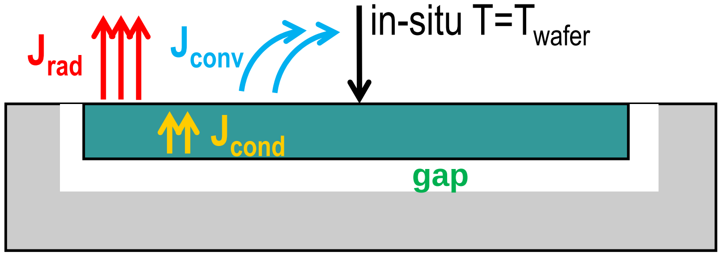
temperature gradient and bow vs wafer and process parameters

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



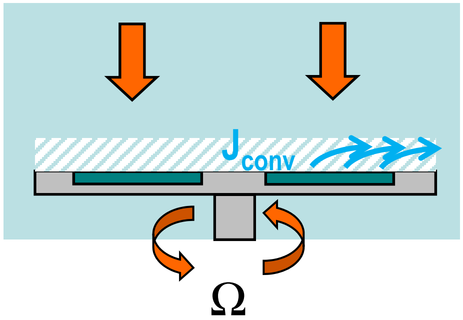
1) Sapphire wafer (*transparent*)



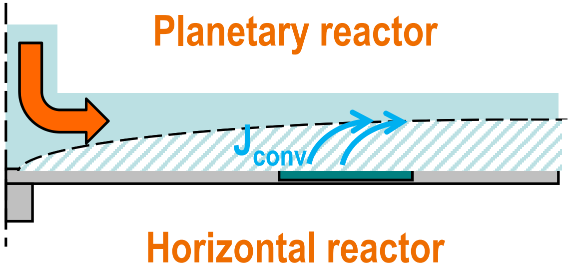
2) Silicon wafer (*opaque*)

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

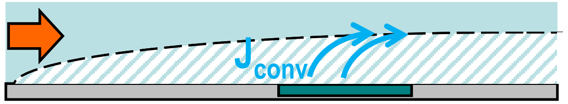
Rotating Disk Reactor



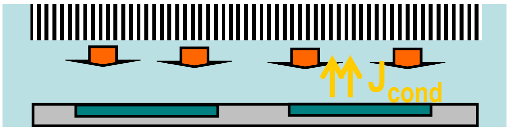
Planetary reactor



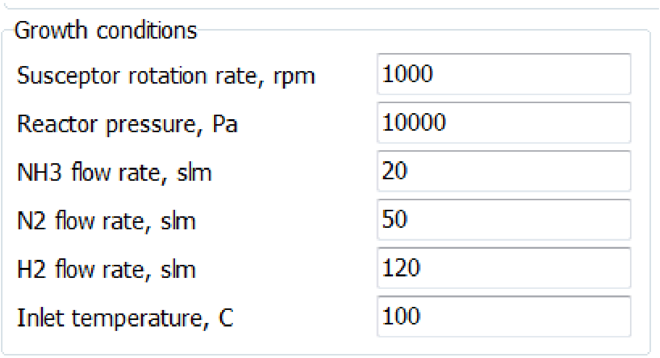
Horizontal reactor



Close coupled showerhead reactor



Wafer bow at the heating stage: effect of wafer size



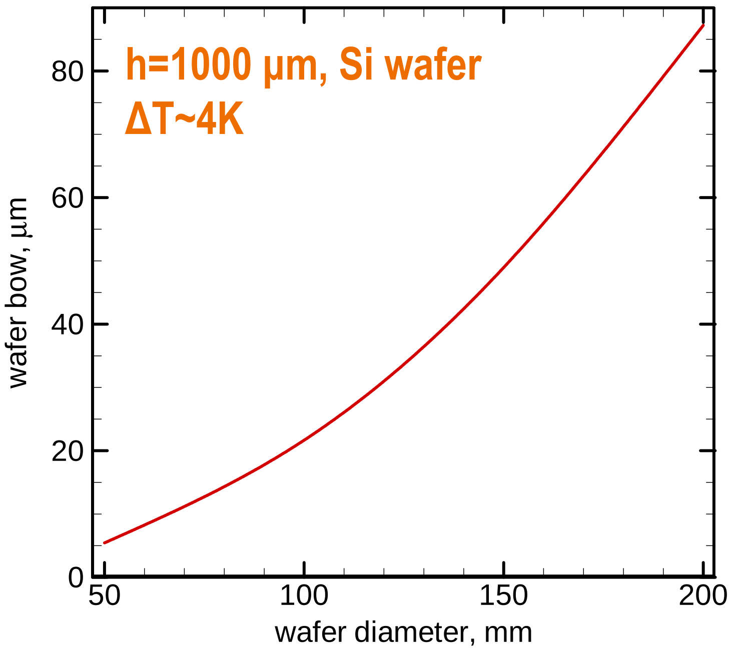
Growth conditions

Susceptor rotation rate, rpm	1000
Reactor pressure, Pa	10000
NH3 flow rate, slm	20
N2 flow rate, slm	50
H2 flow rate, slm	120
Inlet temperature, C	100

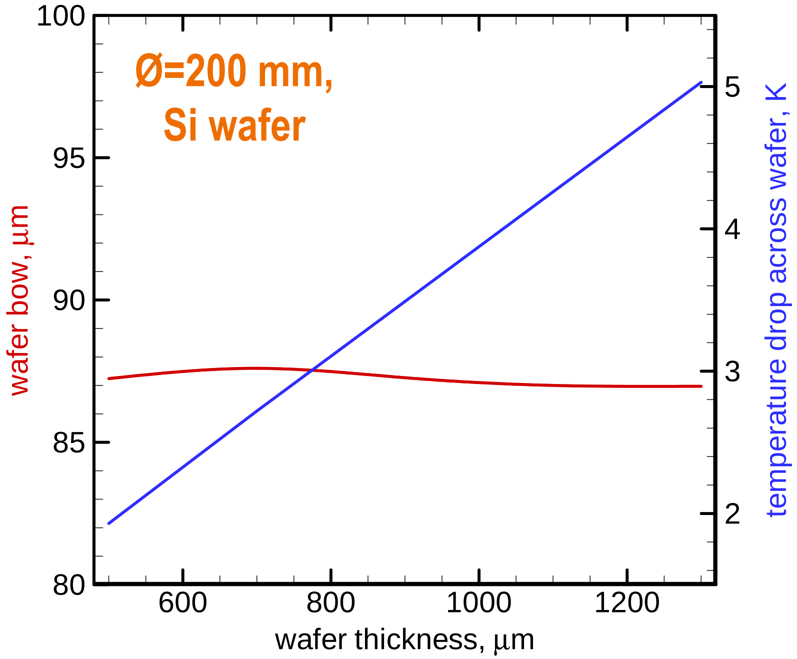
Reactor heating → temperature gradient → wafer bow

Computations take into account:

- substrate radius
- substrate thickness
- substrate initial curvature
- temperature drop is estimated for typical MOCVD reactors



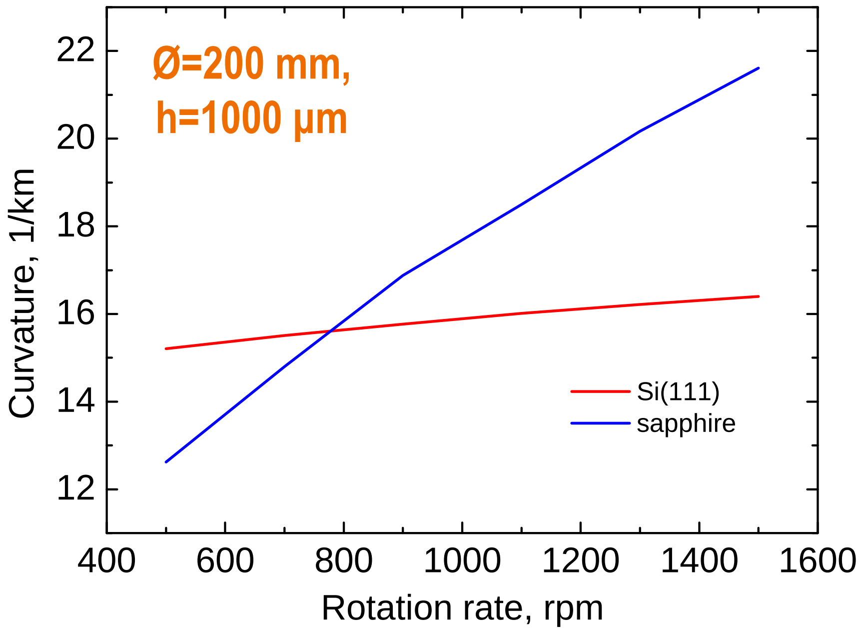
Bow increases with the wafer diameter



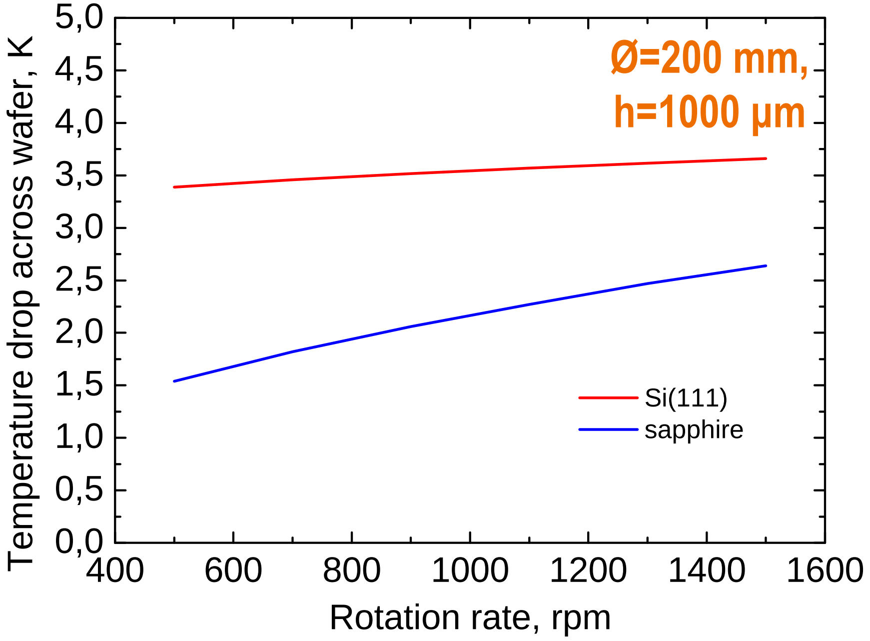
Constant bow: higher ΔT is compensated by higher wafer thickness

Curvature vs process parameters

curvature



temperature drop

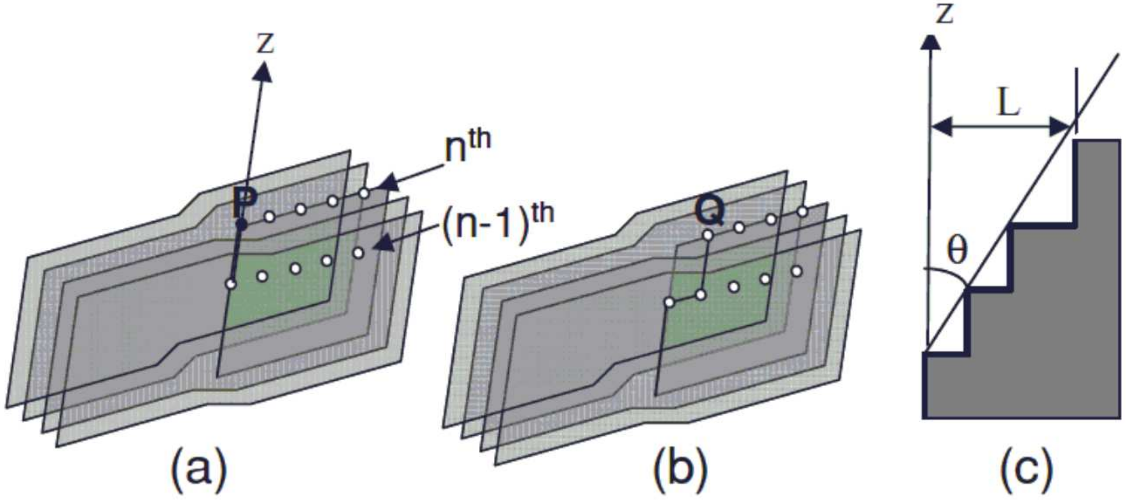


Sapphire wafer is much more sensitive to the variation of the susceptor rotation rate: forced convection provides the largest contribution; for the silicon wafer, radiative heat exchange with the cold plate is important as well

Growth stage:

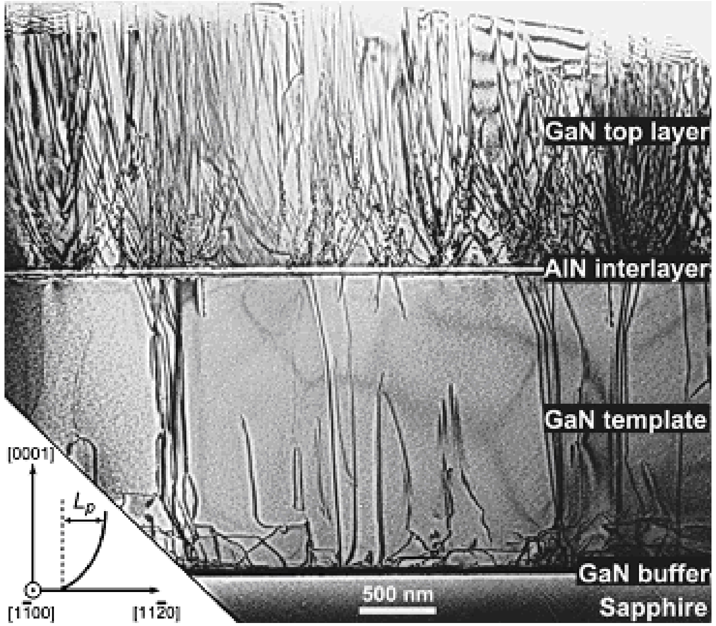
stress, curvature, and dislocation dynamics

Kinetic model of compressive stress relaxation in (Al)GaN layers



- Relaxation of compressive stresses in GaN and AlGaN occurs via inclination of threading dislocations (TD)
- Dislocation inclination occurs only at the growing surface
- For dislocation to incline, atom at the dislocation core needs to get out
- Threading dislocation inclination depends on growth conditions, stress state, surface roughness, and TD density
- Dislocation annihilation is accounted for

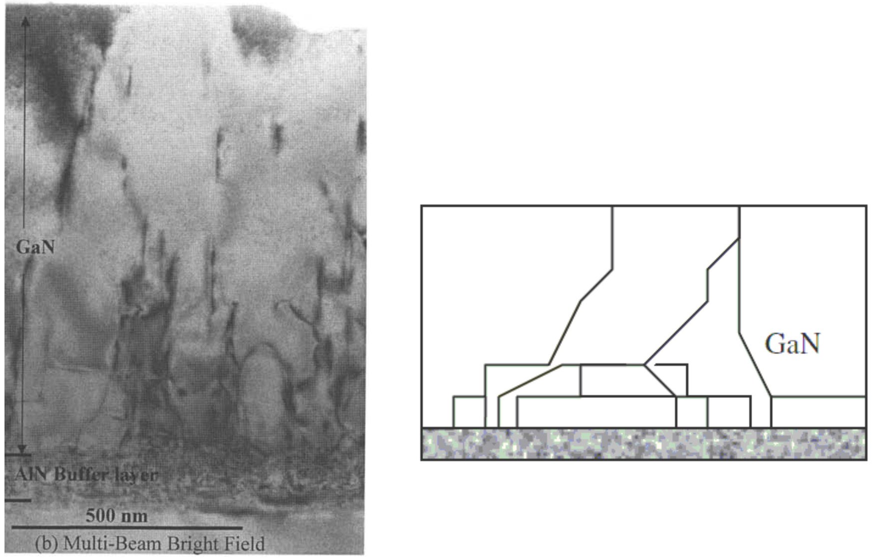
Nucleation and evolution of dislocations in compressively stressed layers



TEM of GaN / AlN IL / GaN structure.

[J.F. Wang. Appl. Phys. Lett. 2006. Vol. 89. 152105]

TD nucleation in compressively strained layers is observed in case of high difference in the composition between top and bottom layers (GaN/AlN)



TEM of GaN film deposited on AlN buffer layers on Si (left) and schematic illustration of large TDs inclination (right).

[S. Raghavan. Appl. Phys. Lett. 2006. Vol. 88. 041904.] and
[S. Raghavan. J. Cryst. Growth. 2012. Vol. 359. Pp. 35–42]

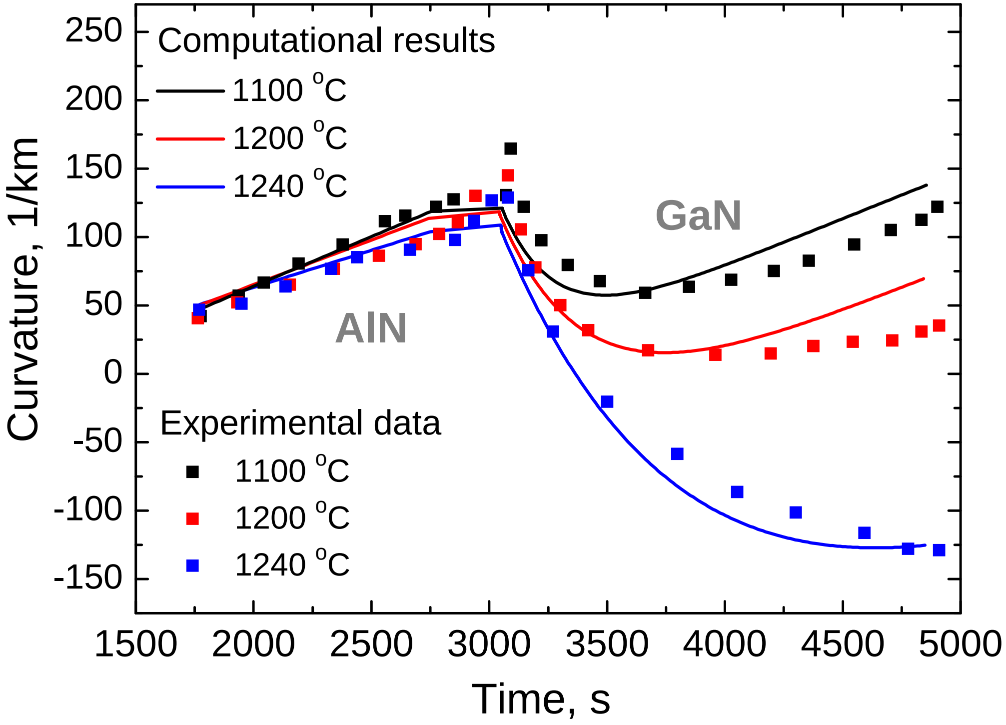
Sharp reduction of the TDD close to the GaN/AlN interface is attributed to large inclination and annihilation of the TDs

The net compressive stress at which the GaN layers start growing on Al(Ga)N buffer is always about −1 to −1.7 GPa and does not increase even in case of GaN on AlN buffer.

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}~6.0·10^{10}

ρ_{TD}~3.8·10^{10}

ρ_{TD}~1.8·10^{10}

Wafer: Si, 50 mm

Purpose: high quality AlN for GaN/Si growth

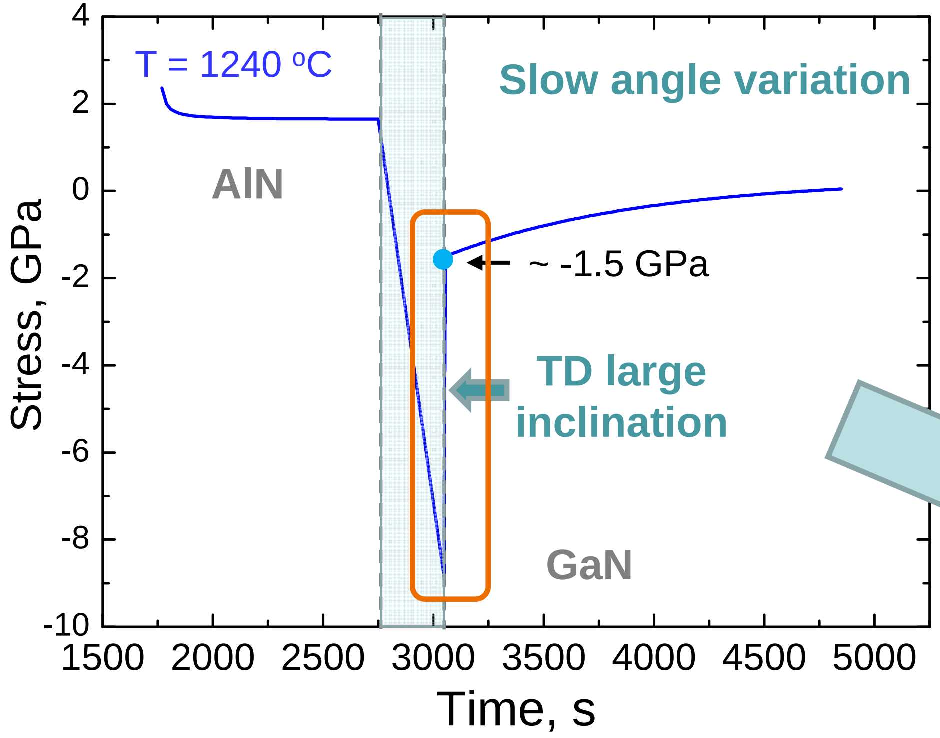
Structure: (115nm) AlN / (1.7μm) GaN

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

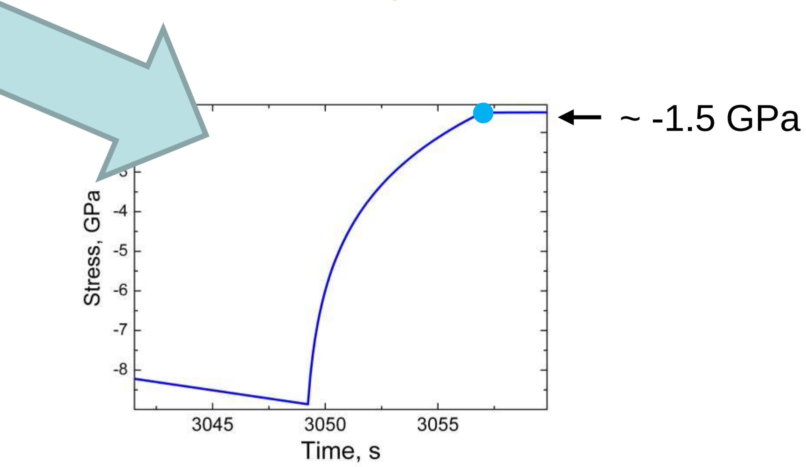
Evolution of stress in GaN/AlN structure: modeling

Wafer: Si, 50 mm
Purpose: high quality AlN for GaN/Si growth
Structure: (115nm) AlN / (1.7µm) GaN

AlN quality (dislocation density) is a function of the growth temperature



Rapid relaxation of the mismatch stress at the initial stage of GaN growth occurs via large inclination of pre-existing and nucleated threading dislocations. Correspondingly, the stress rapidly changes to about -1.5 GPa

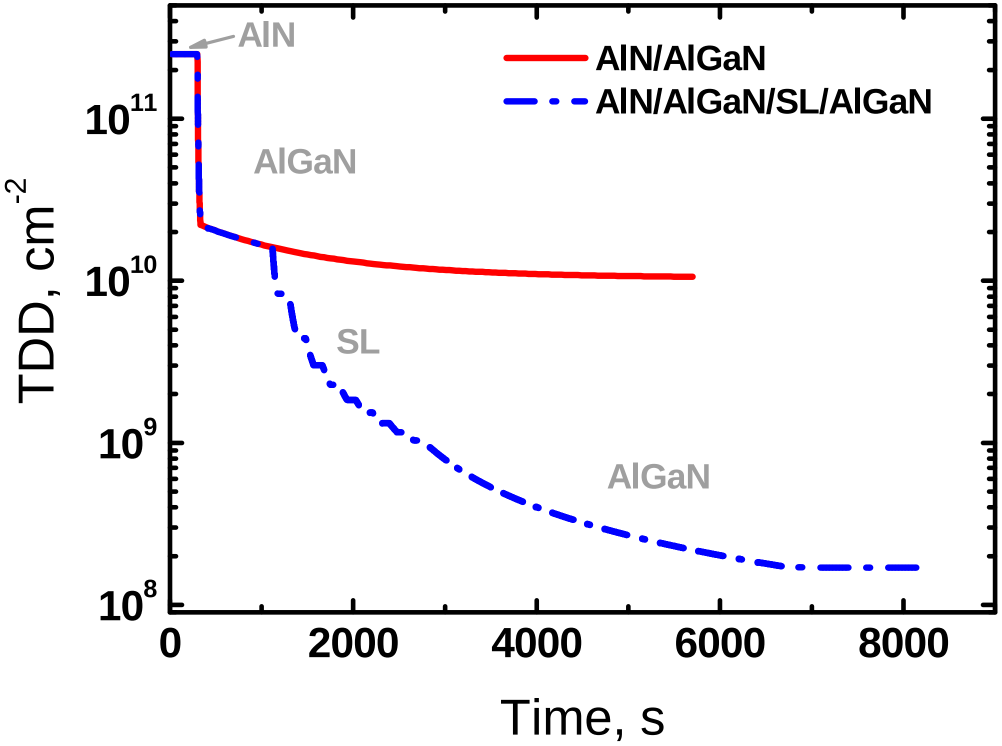


C. Liu et al., Phys. Stat. Sol. C 10, 11 (2013) 1541

Application of superlattice (SL) as dislocation filter

Wafer: Al_2O_3, 50 mm
Purpose: thick high quality AlGaN layers for DUV active region
Structure: AlN/$Al_{0.2}Ga_{0.8}N$ + SL in-between:
10-period (8nm) AlN / (24nm) AlGaN

Strong reduction of the dislocation density when SL is used



Measurements:
ρ_{TD}~$1.0 \cdot 10^{10}$
ρ_{TD}~$2.5 \cdot 10^{8}$

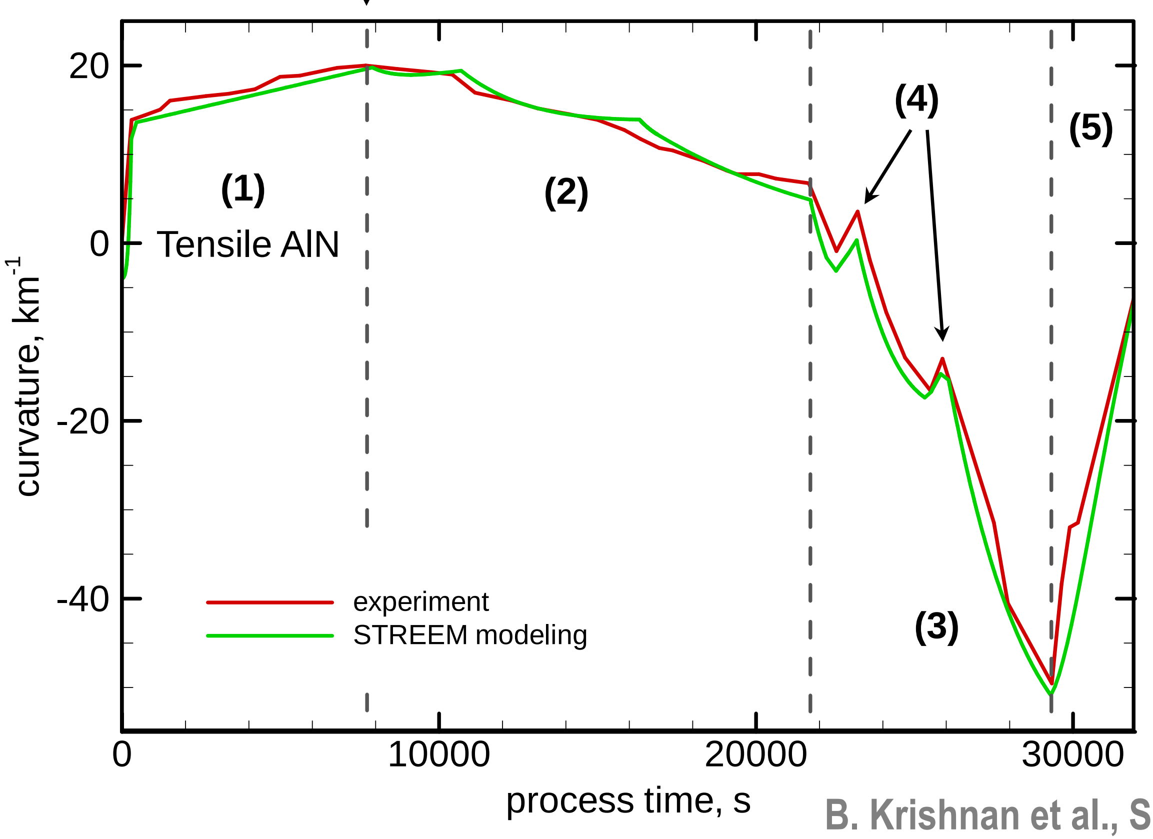
Partial relaxation of the AlN layers in the SL structure continuously introduces compressive stress in the subsequent AlGaN layers, which provides large inclination of the threading dislocations and acceleration of their annihilation

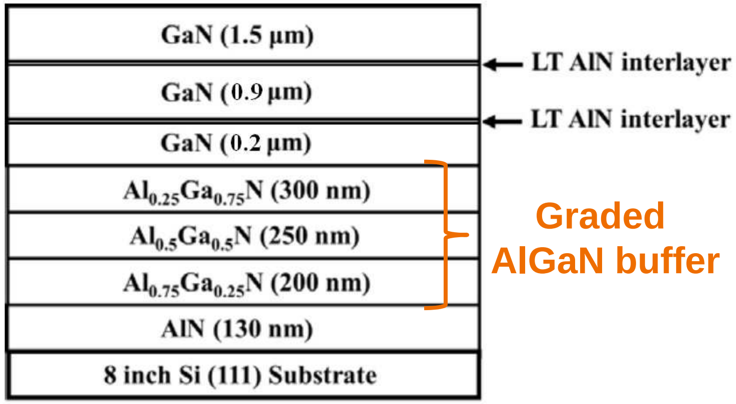
J.P. Zhang et al., Appl. Phys. Lett. 80, 19 (2002) 3542

Use of AlGaN graded buffers for strain engineering

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

TDD was specified here




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

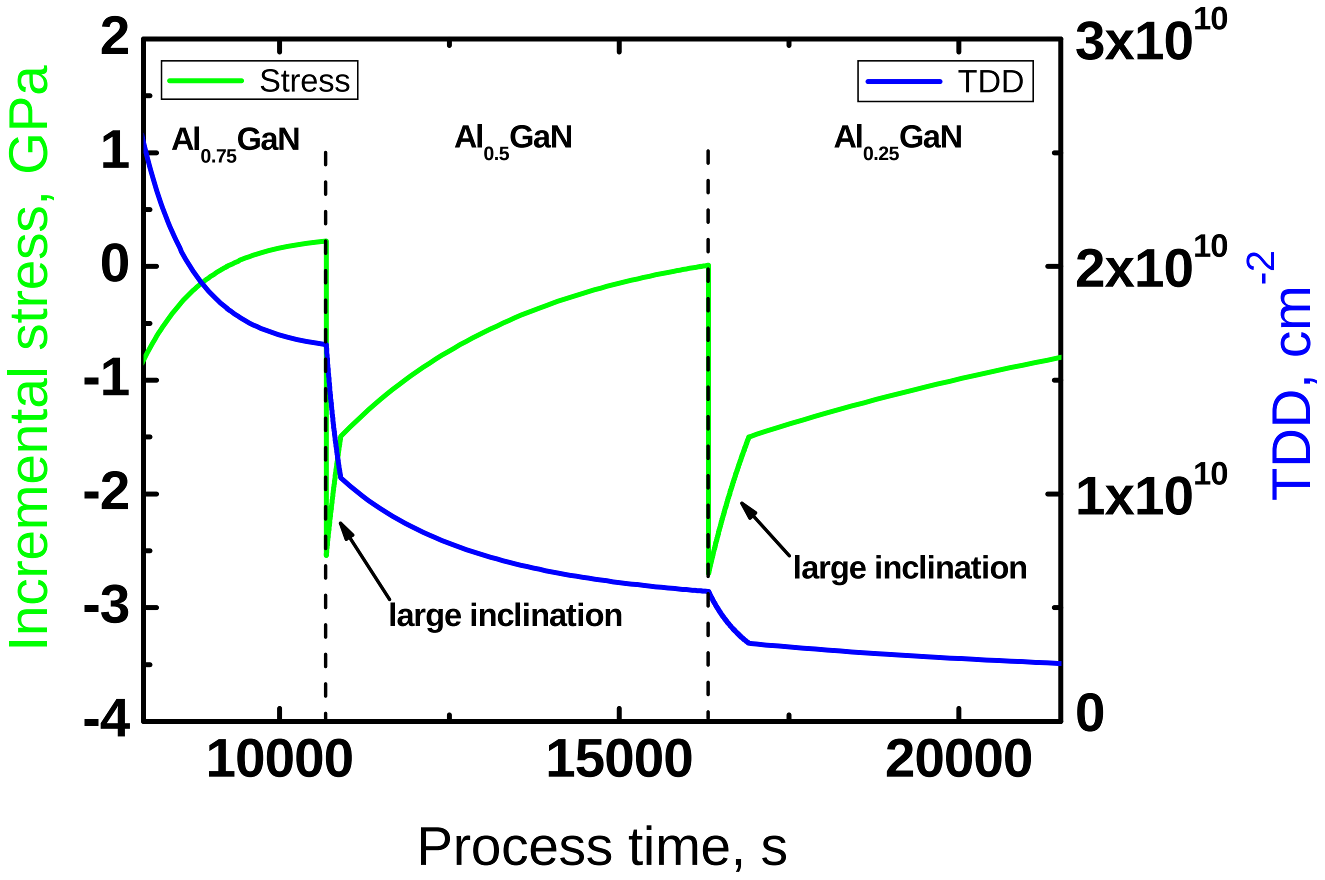
Graded AlGaN buffer

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



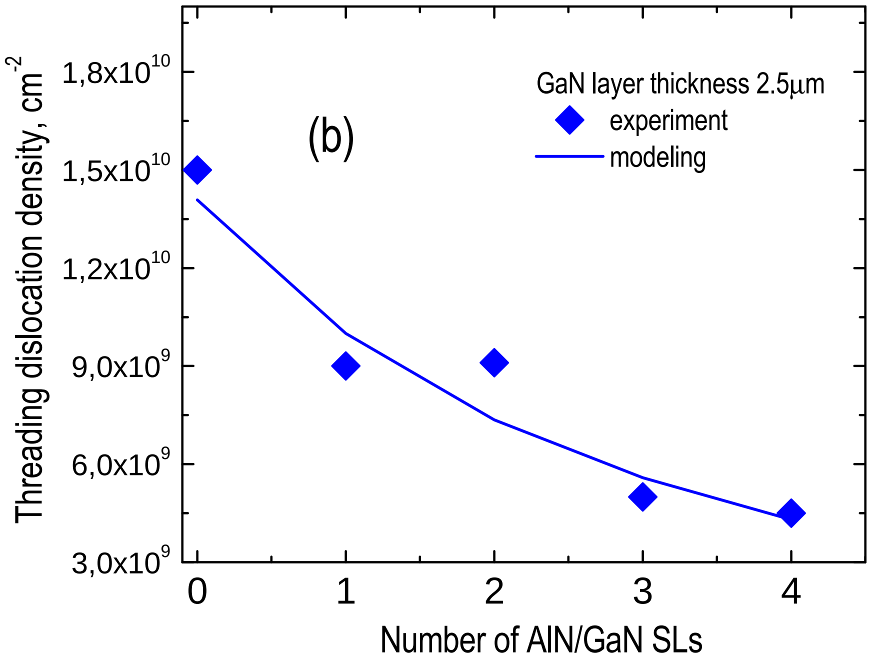
Closer look at the graded AlGaN buffer shown also in segment (2) of the plot on the previous page

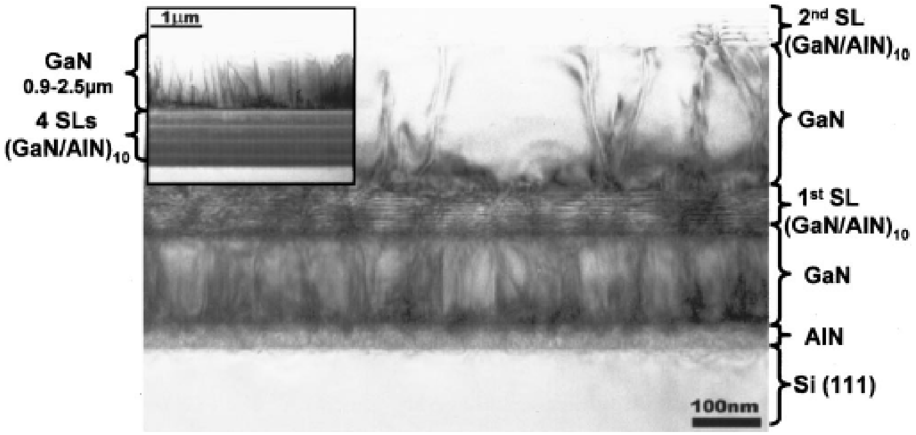
Gradual decrease of the dislocation density, ultimately, by an order of magnitude, in the graded AlGaN buffer.
Large inclination of the threading dislocation due to high mismatch stress

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

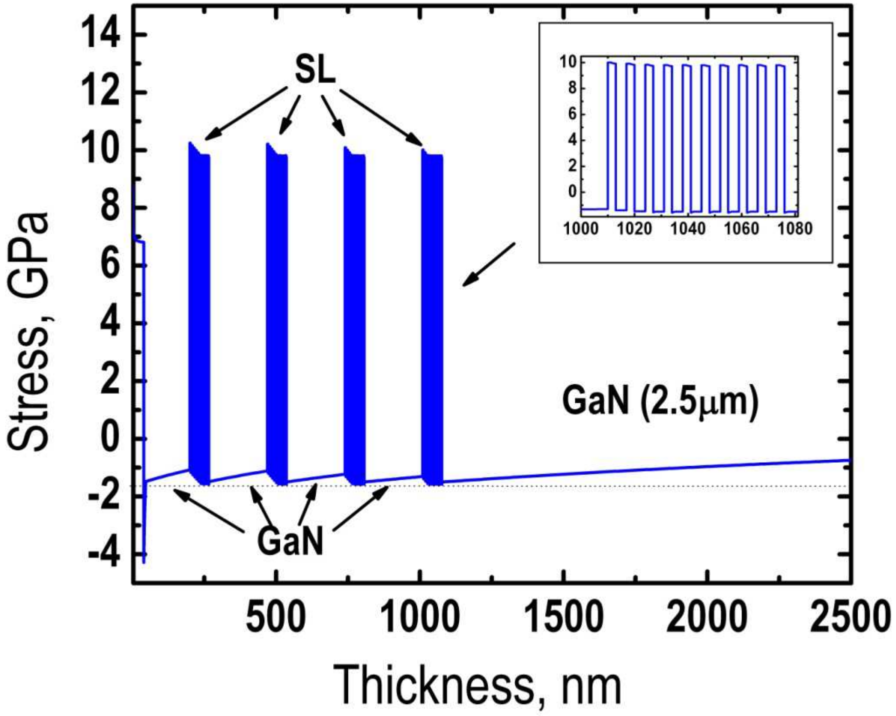


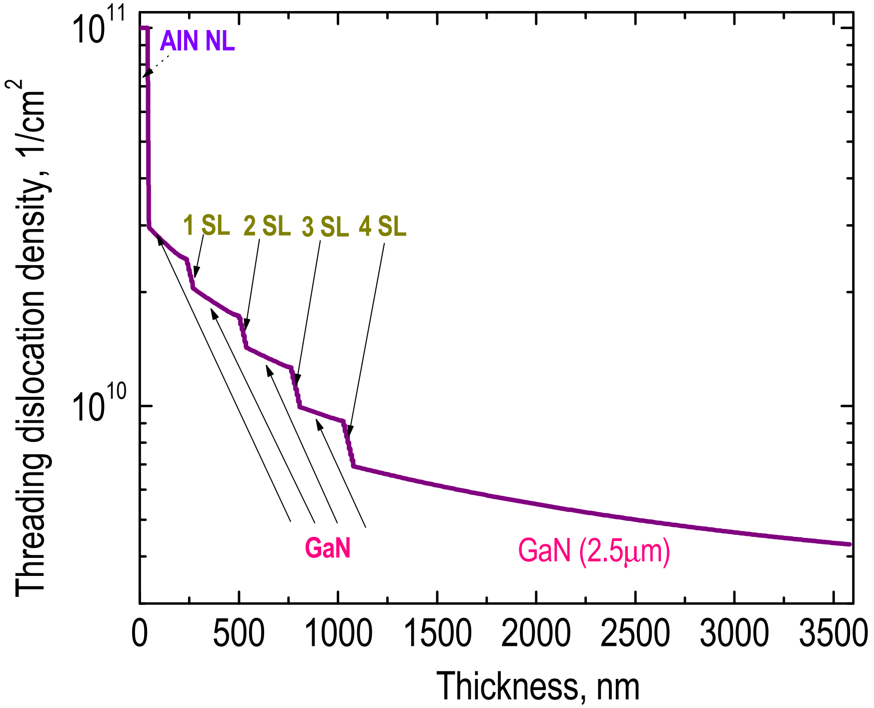


- ✓ Superlattices can efficiently counteract the tensile stress usually observed in GaN on Si
- ✓ Reduction of the dislocation density with the number of SLs
- ✓ Crack-free 2.5 µm thick GaN can be grown on this buffer structure

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

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





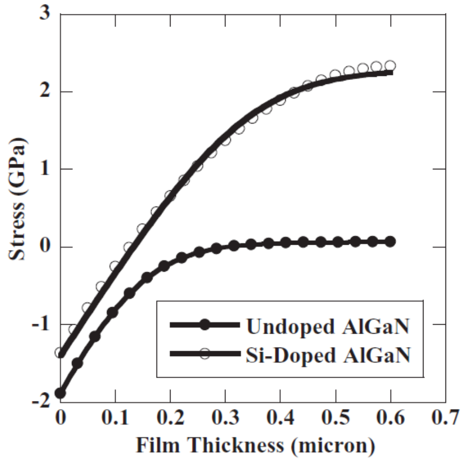
- high stress in the first GaN layer results in nucleation of new dislocations and fast reduction of their density due to large inclination and annihilation.
- thin AlN layers in the SLSs are far from being fully relaxed.
- formation of new dislocations in GaN layers is not predicted. Instead, the dislocation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

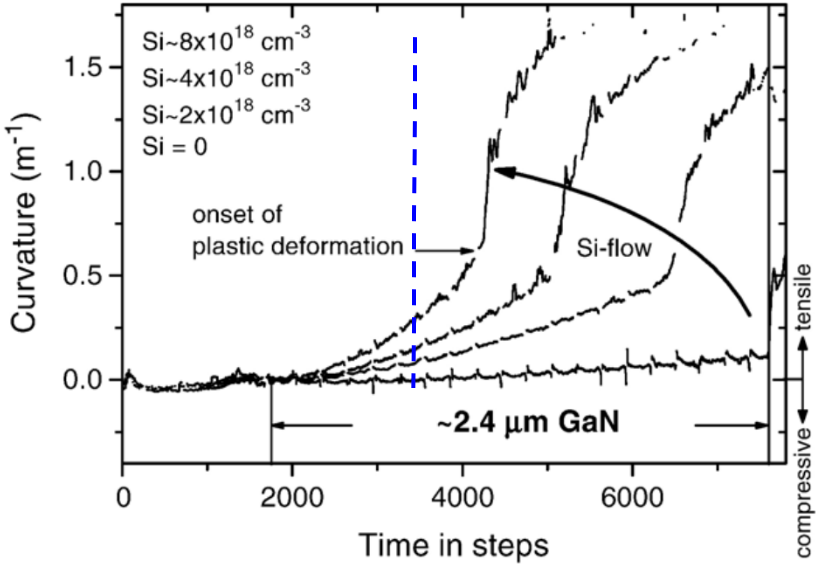
E. Feltin et al., Appl. Phys. Lett. 79 (2001) 3230

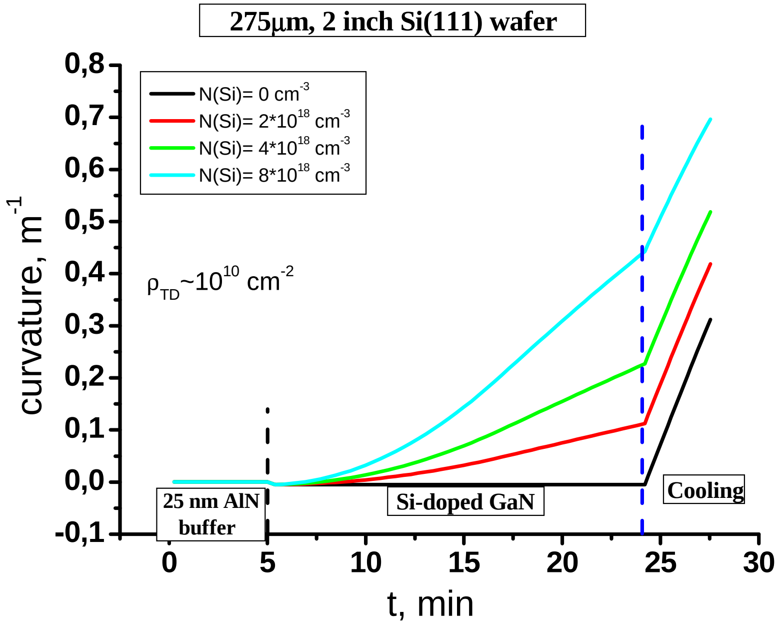
Effect of Si doping on stress evolution

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;







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

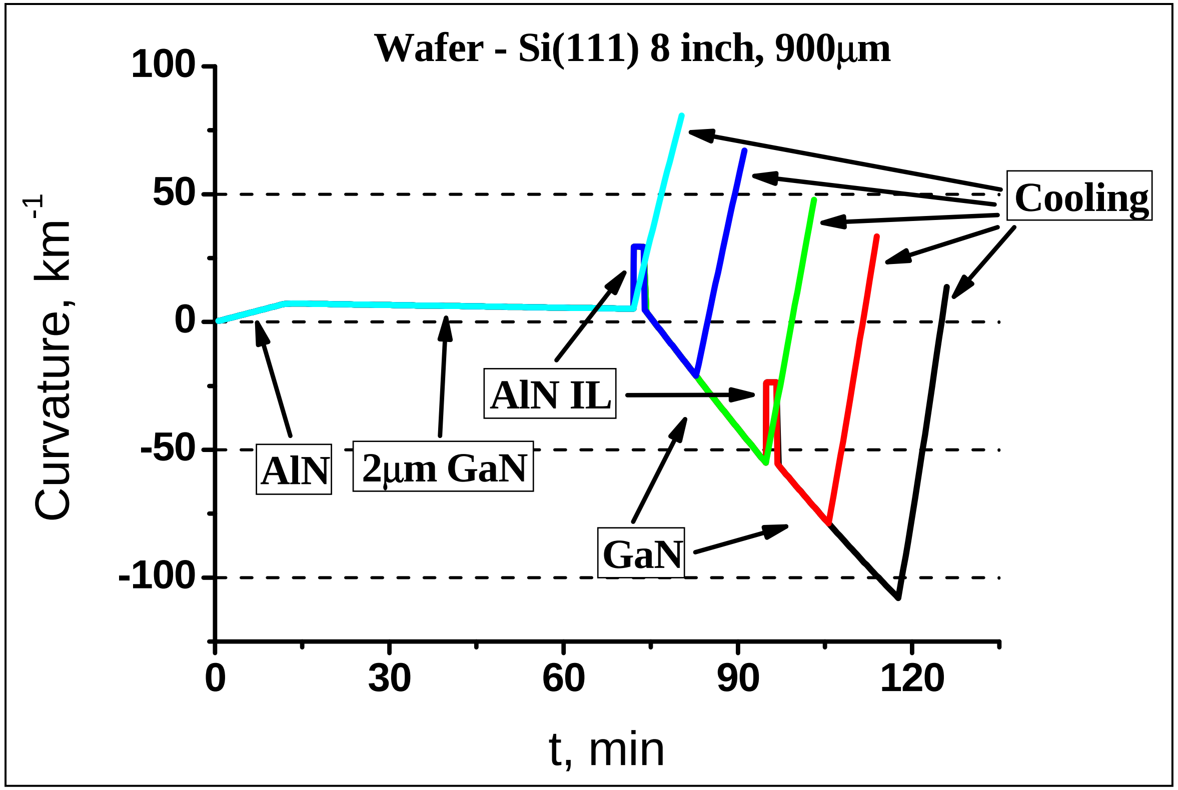
Structure cooling:

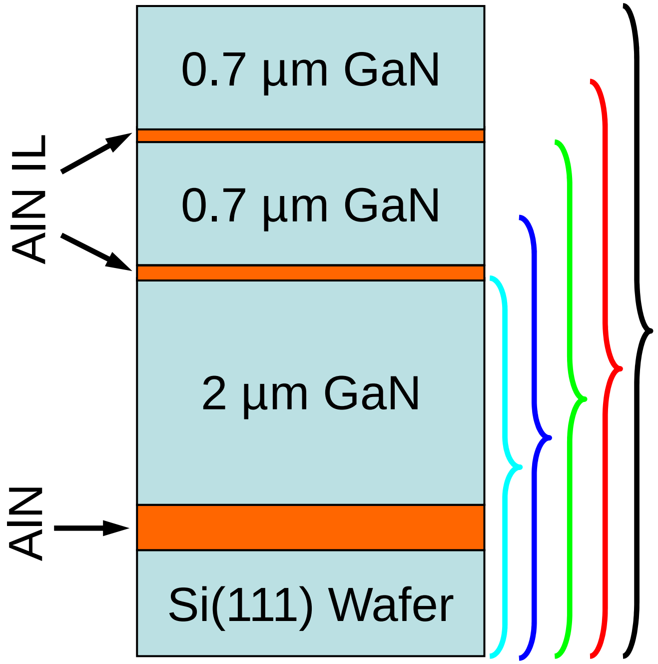
stress, bow, cracking

Prediction of bowing @RT

Prediction of bowing @RT

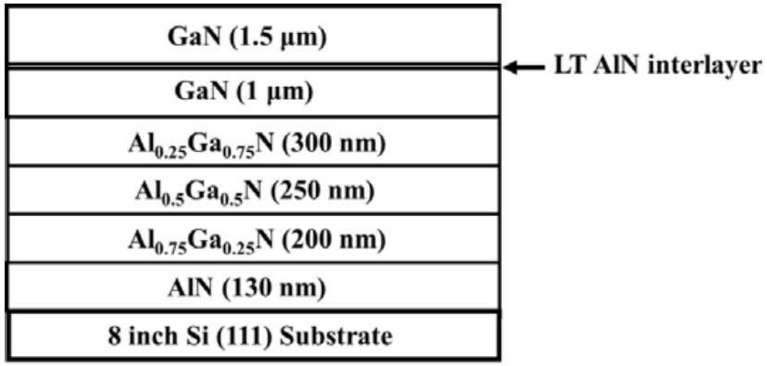
- In case the curvature evolution for the whole structure is known and bowing at room temperature is not zero, it is possible to find optimal position to stop the process, cool the structure, and expect zero curvature at RT

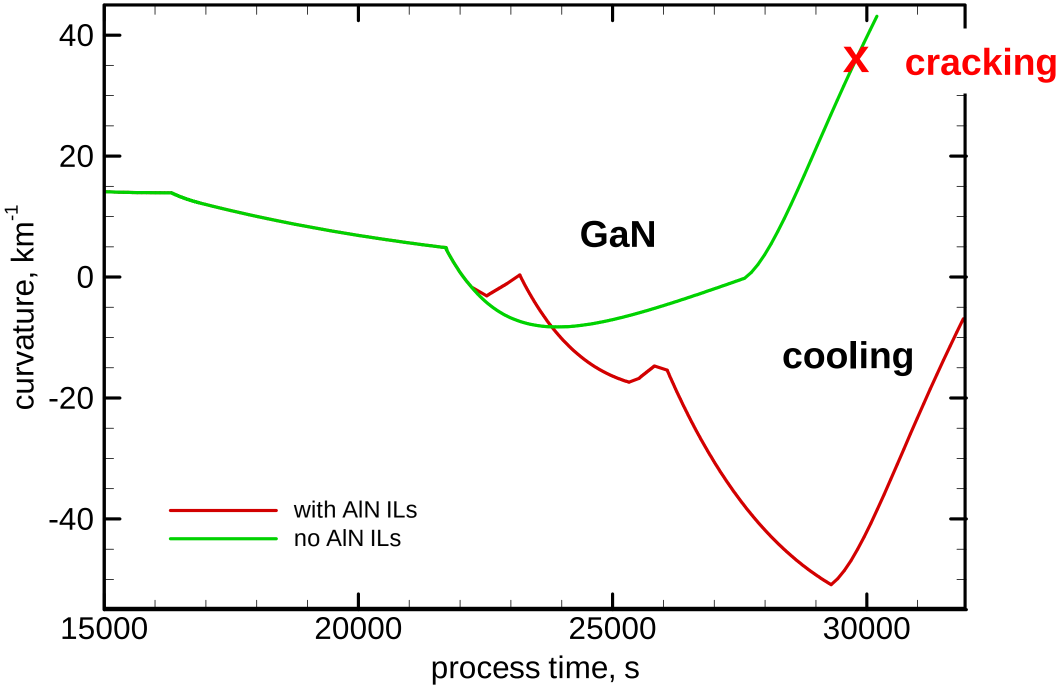




Insertion of AlN ILs at the stage of thick GaN growth

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



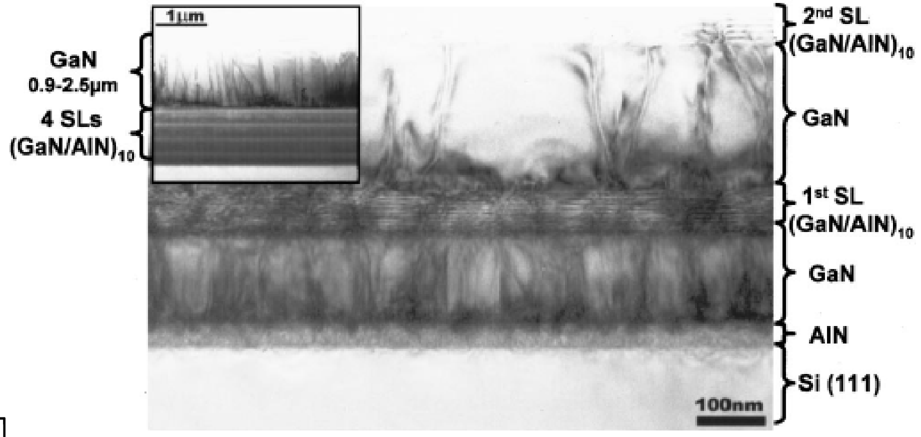


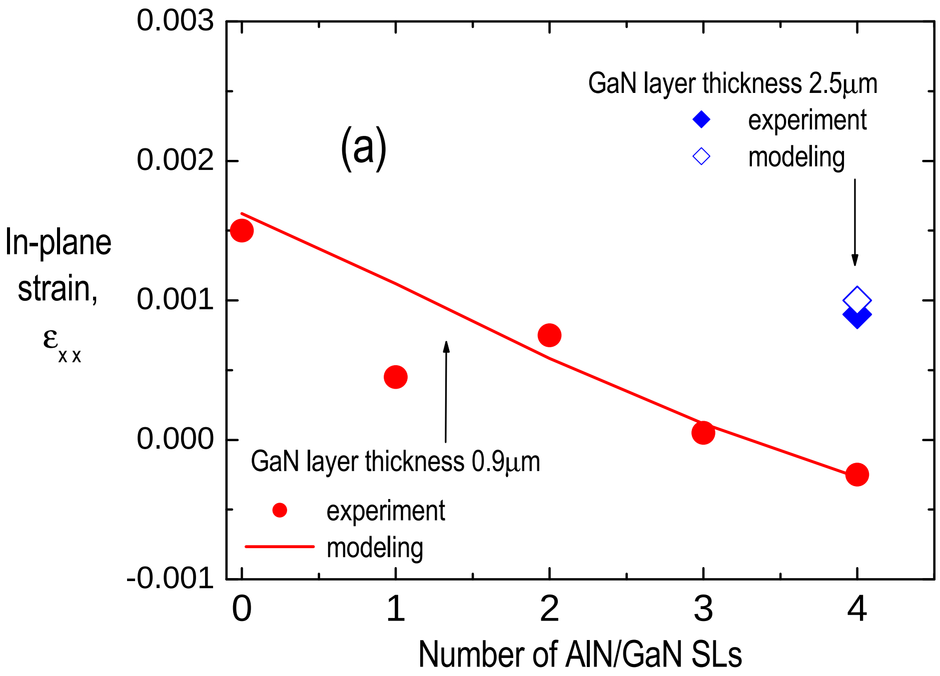
When AlN intelayers do not introduce additional compressive stress into the structure, cracked structure is predicted after cooling

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

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





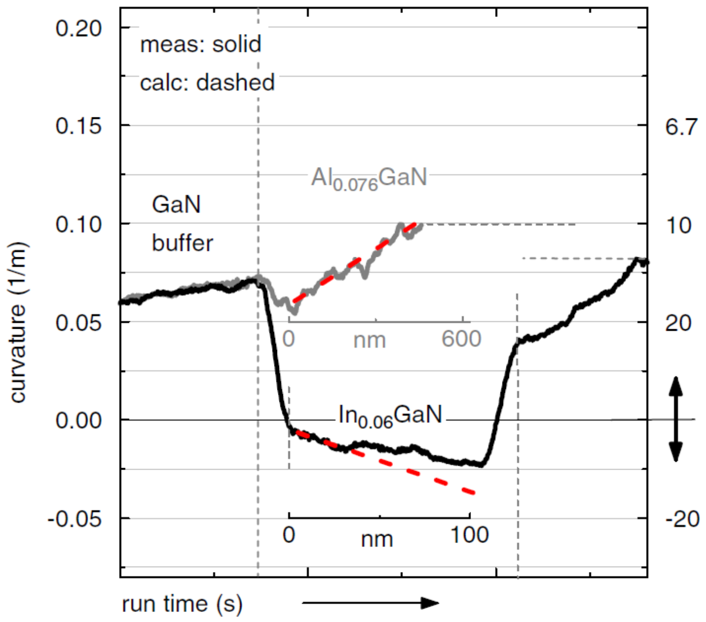
About linear decrease of the in-plane strain of the GaN layers with the number of superlattices used in the structure is reproduced well by the modeling

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

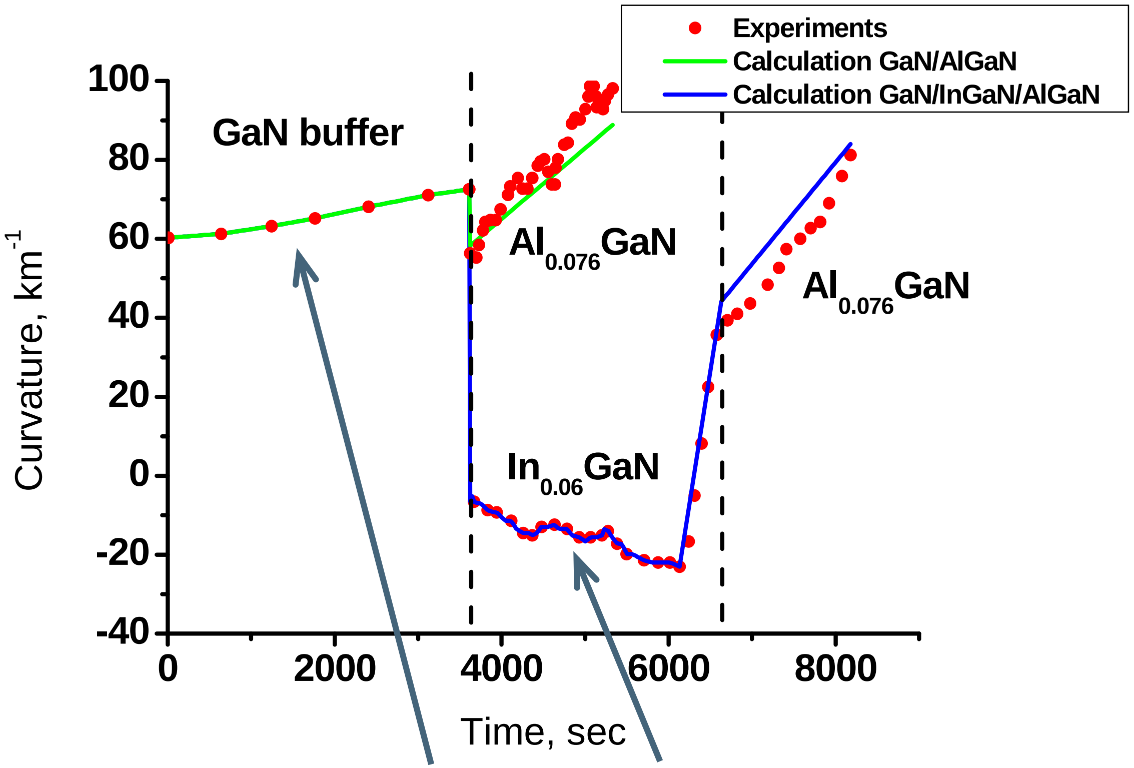
Inverse problem

and curvature modeling

Use of extracted stress evolution for curvature modeling



Experimental curvature evolution during growth of GaN/AlGaN and GaN/InGaN/AlGaN structures on 340µm Sapphire substrate.



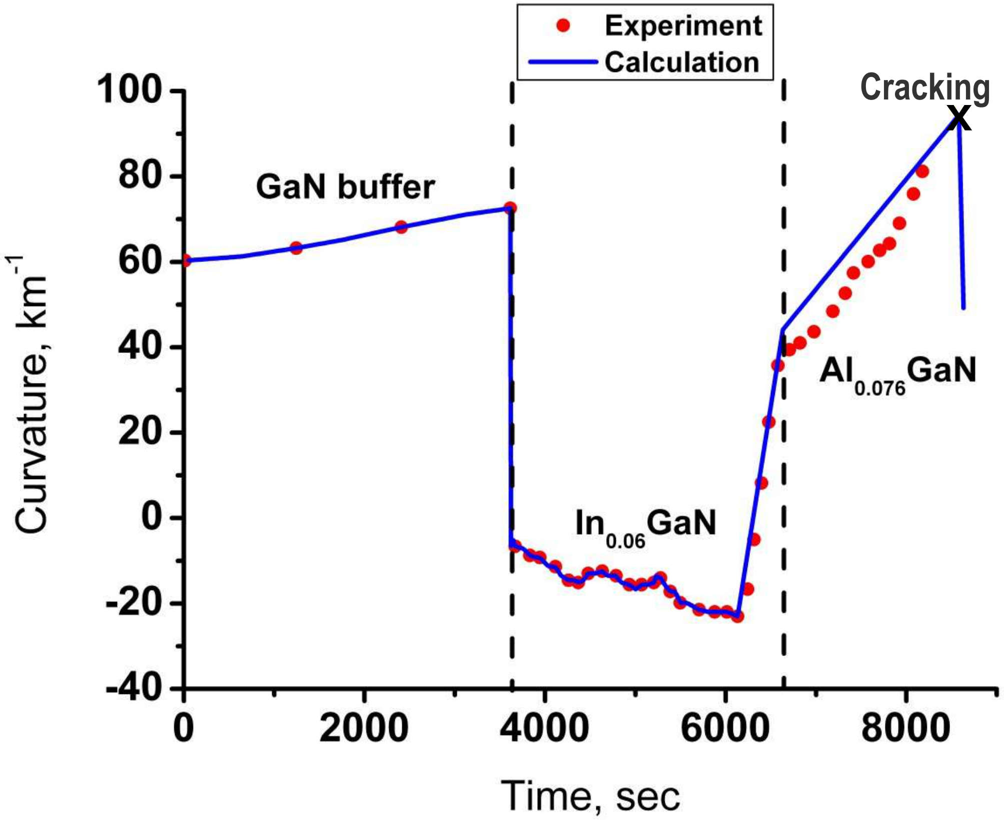
Simulation mode: Experimental Stress Evolution

- **Inverse problem solution allows to achieve experimental stress evolution in the structure**
- **The extracted stress evolution can be used for the initial stages during modeling of curvature evolution of more complex structure**

F. Brunner et al., J. Crystal Growth 298 (2007) 202-206

Here the extracted stress evolution is used for curvature modeling for GaN buffer in GaN/AlGaN structure (green line) and for GaN buffer and InGaN layer in GaN/InGaN/AlGaN structure (blue line).

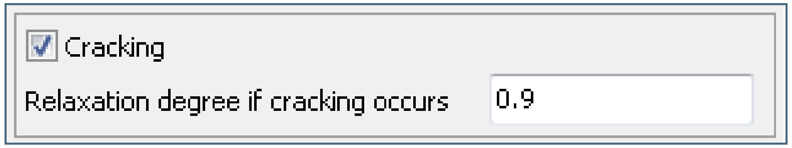
Prediction of cracking during structure growth



- Layer cracking during growth continuation is predicted by STREEM-AlGaN

- Degree of possible stress relaxation via layer cracking is specified by user

Here extracted stress evolution is used for curvature modeling for GaN buffer and InGaN layer in GaN/InGaN/AlGaN structure.


☑ Cracking

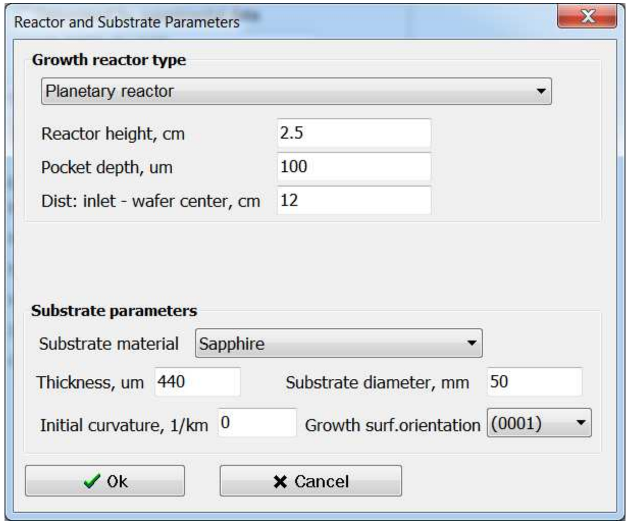
Relaxation degree if cracking occurs 0.9

F. Brunner et al., J. Crystal Growth 298 (2007) 202-206

STREEM-AlGaN:

software interface and operation

Wafer parameters and reactor type



Reactor and Substrate Parameters

Growth reactor type

Planetary reactor

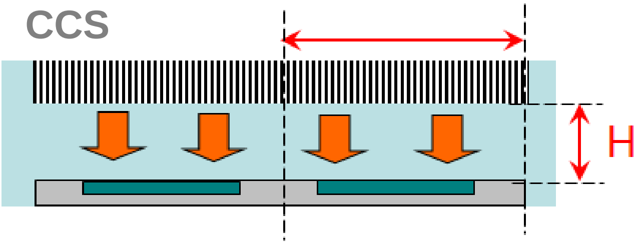
Reactor height, cm: 2.5
Pocket depth, um: 100
Dist: inlet - wafer center, cm: 12

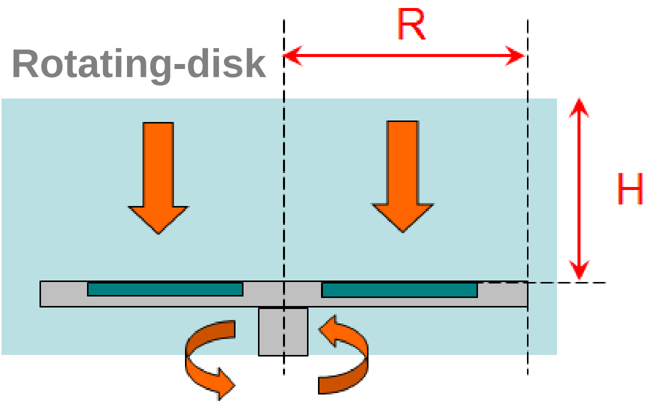
Substrate parameters

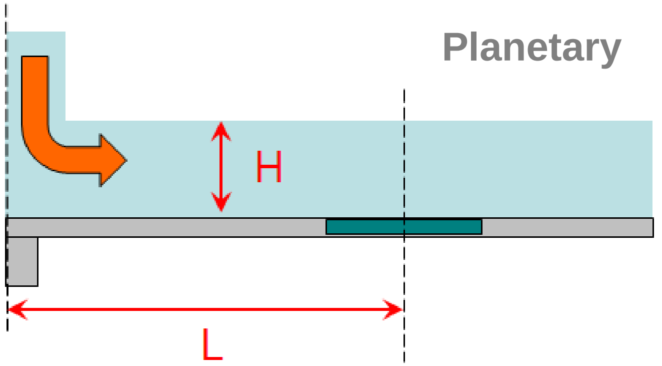
Substrate material: Sapphire
Thickness, um: 440
Substrate diameter, mm: 50
Initial curvature, 1/km: 0
Growth surf.orientation: (0001)

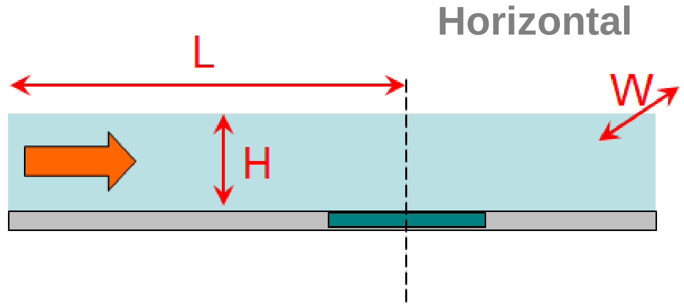
Reactor geometrical parameters (optionally) to estimate the temperature drop from process conditions

Wafer diameter, thickness, and initial curvature



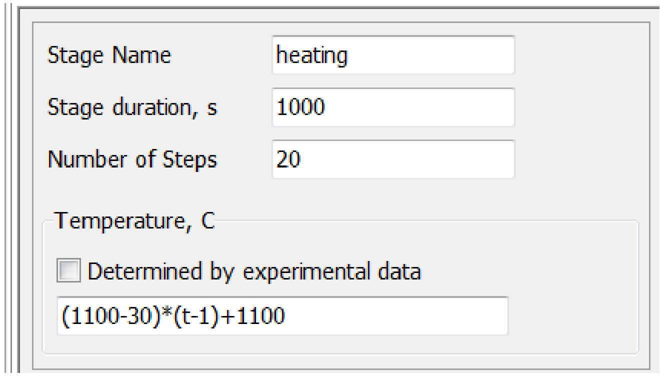






Specification of the process stages

Heating/cooling



Stage Name	heating
Stage duration, s	1000
Number of Steps	20

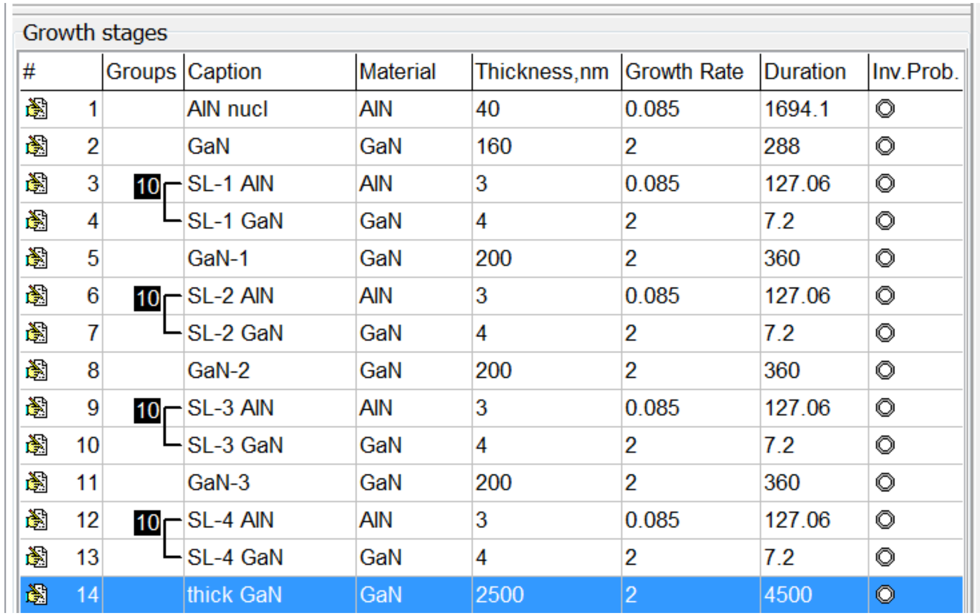
Temperature, C

☐ Determined by experimental data

(1100-30)*(t-1)+1100

Duration + law of temperature variation (e.g., linear)

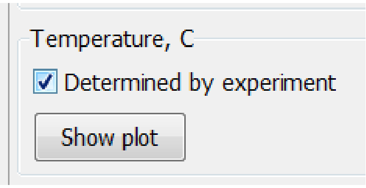
Growth stages



Growth stages

#	Groups	Caption	Material	Thickness,nm	Growth Rate	Duration	Inv.Prob.
1		AlN nucl	AlN	40	0.085	1694.1	○
2		GaN	GaN	160	2	288	○
3	10	SL-1 AlN	AlN	3	0.085	127.06	○
4		SL-1 GaN	GaN	4	2	7.2	○
5		GaN-1	GaN	200	2	360	○
6	10	SL-2 AlN	AlN	3	0.085	127.06	○
7		SL-2 GaN	GaN	4	2	7.2	○
8		GaN-2	GaN	200	2	360	○
9	10	SL-3 AlN	AlN	3	0.085	127.06	○
10		SL-3 GaN	GaN	4	2	7.2	○
11		GaN-3	GaN	200	2	360	○
12	10	SL-4 AlN	AlN	3	0.085	127.06	○
13		SL-4 GaN	GaN	4	2	7.2	○
14		thick GaN	GaN	2500	2	4500	○

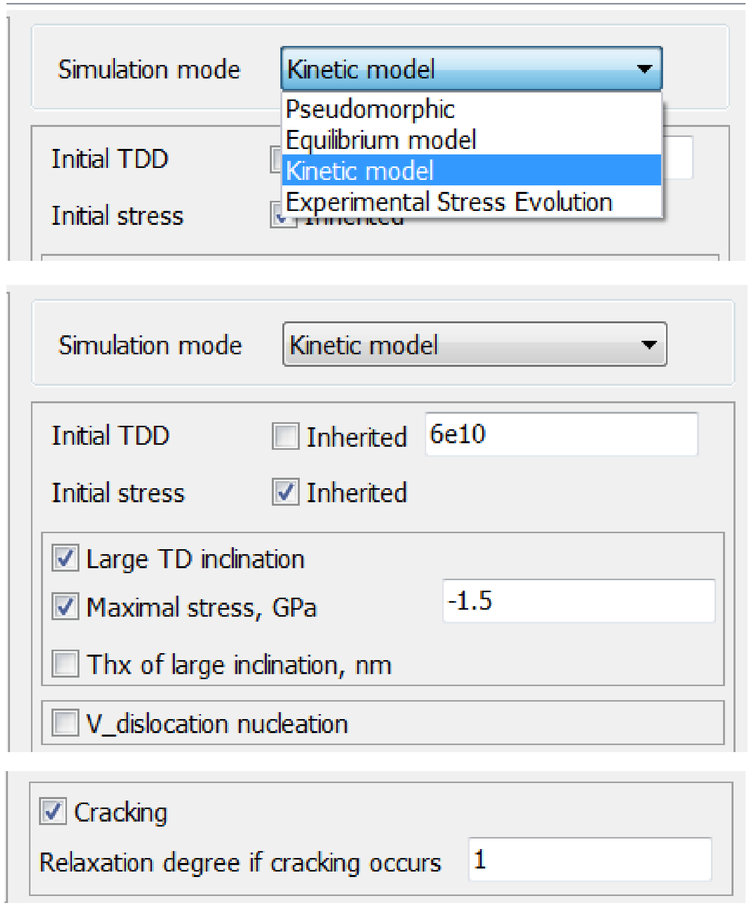
- ✓ Conventional parameters: duration, thickness, temperature
- ✓ Process parameters (optionally) to estimate the temperature drop
- ✓ Ability to group several stages that are repeated more than once in the recipe
- ✓ Ability to use *in-situ* temperature measurements as process parameter with graphical representation



Temperature, C

☑ Determined by experiment

Simulation modes



Simulation mode: Kinetic model

Initial TDD

Initial stress

Simulation mode: Kinetic model

Initial TDD ☐ Inherited 6e10

Initial stress ☑ Inherited

☑ Large TD inclination

☑ Maximal stress, GPa -1.5

☐ Thx of large inclination, nm

☐ V_dislocation nucleation

☑ Cracking

Relaxation degree if cracking occurs 1

✓ **Pseudomorphic growth**

$$\varepsilon_1 = \frac{a_1^{eff}(T_1) - a_1(T_1)}{a_1(T_1)}, \text{ generalized for stack of layers}$$

✓ **Equilibrium model**

$$\rho_{MD_i}(C_i^R) = \rho_{MD_i}^{equil.} \cdot C_i^R$$

C_i^R degree of relaxation

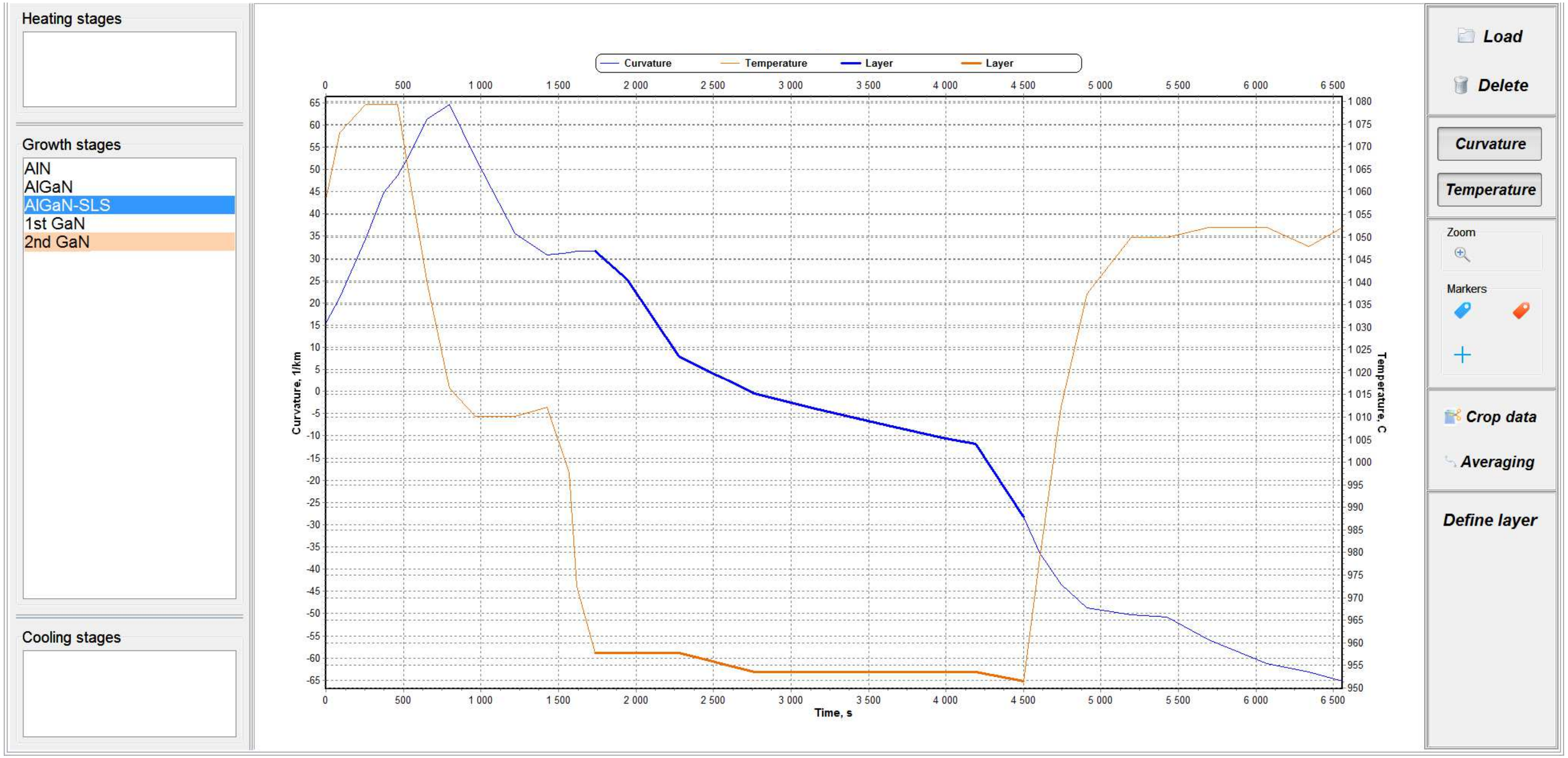
Dodson-Tsao dependence for equilibrium relaxation

✓ **Kinetic model**

- **inclination of the existing dislocation for compressively stressed layers (grading AlGaN)**
- **nucleation and large inclination of dislocations for heavily mismatched layers (GaN/AlN)**

✓ **Cracking of the layers under tensile stress**

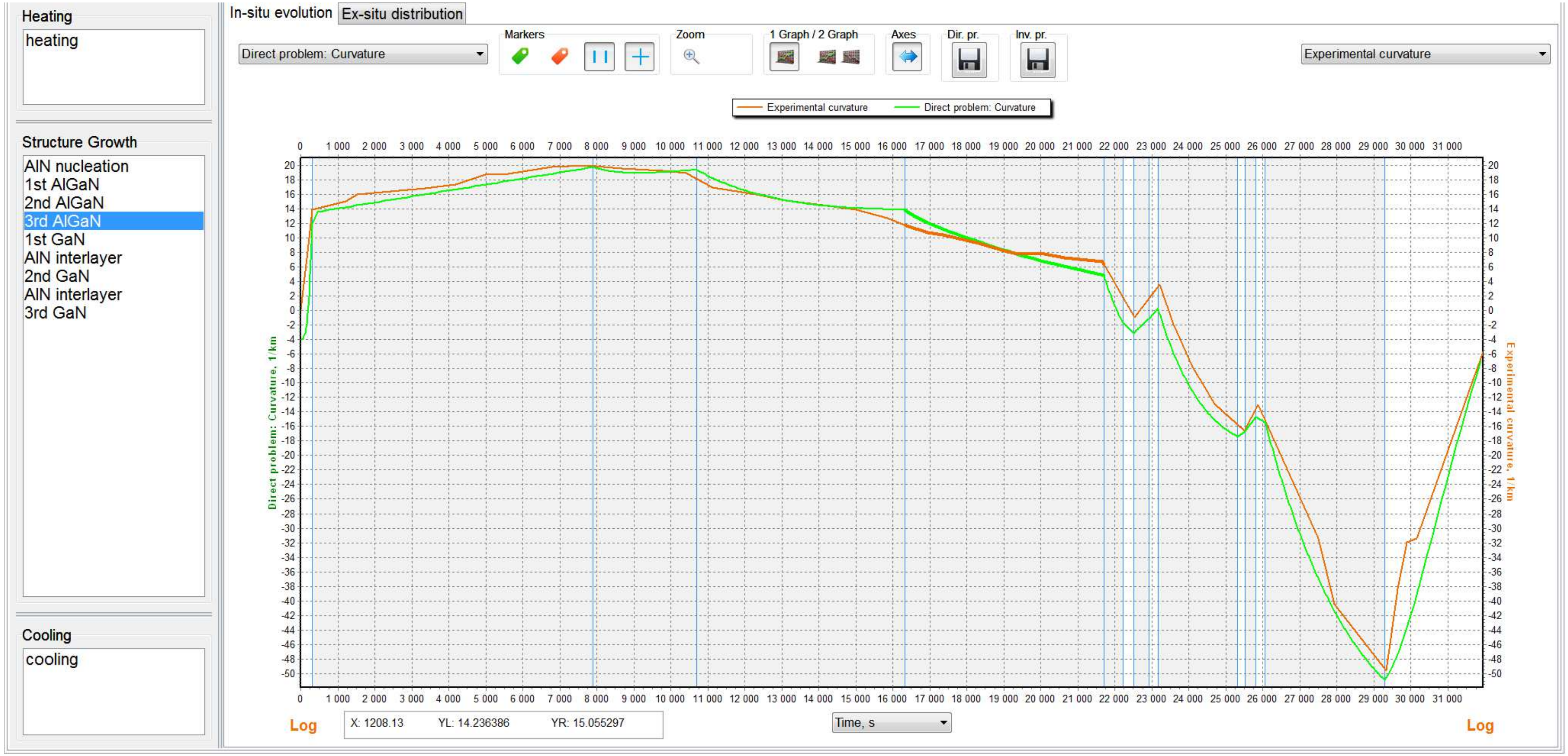
Loading of in-situ measurements



AlN
AlGaN
AlGaN-SLS
1st GaN
2nd GaN

- ✓ Available for curvature and temperature;
- ✓ Can be used to (1) set measured temperature as process parameter; (2) use the curvature data for comparison with model predictions; (3) to solve inverse problem;
- ✓ Ability to specify the stage durations on the *in-situ* curves

Visualization of the results



Direct problem: Curvature

Experimental curvature

X: 1208.13 YL: 14.236386 YR: 15.055297

- ✓ *in-situ* evolution of the stress, bow, curvature, TDD, and critical stress for cracking;
- ✓ ex-*situ* distributions of the stress and effective lattice constant;
- ✓ highlighting of the process stages on the plot;
- ✓ point probe and markers;
- ✓ comparison with experimental data