Investigation of growth mode in AlN buffer layer for strain and dislocation control in Al-rich AlGaN using hot-wall MOCVD

Pitsiri Sukkaew [1,2], Karl Rönnby [2], Jr-Tai Chen [1,2], Henfang Zhang [1,2], Lars Ojamäe [2] and Vanya Darakchieva [1,2]

[1] Center for III-Nitride Technology (C3NiT-Janzén), [2] Department of Physics, Chemistry and Biology (IFM), Linköping University, Sweden

Challenges in the growth of Al-rich AlGaN

- Heteroepitaxy of AlGaN at low temperature produces surface morphology dominated by screw dislocations. Increasing temperature or decreasing thickness can improve the roughness, while increasing the strain which may lead to crack formation during the cooling down. The best strategy in improving the AlGaN is thus via improving the AlN buffer.
- **In this work,**
  - ✓ **We show the experimental results on the effects of AlN buffer on AlGaN in terms of strains and dislocations.**
  - ✓ **We present a CVD kinetic model of AlN which directly links the dislocation densities to the AlN growth temperatures. We show that it is the adsorption-site preference of the growth species (Al and AlH) that acts as a direct factor in controlling AlN growth mode.**

Gas-phase model of AlN CVD

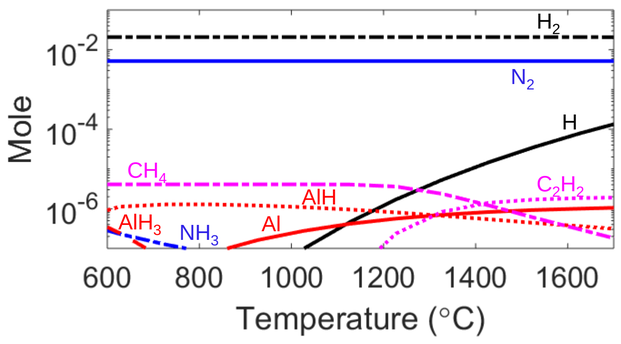
Methods

Gas-phase kinetic model contains

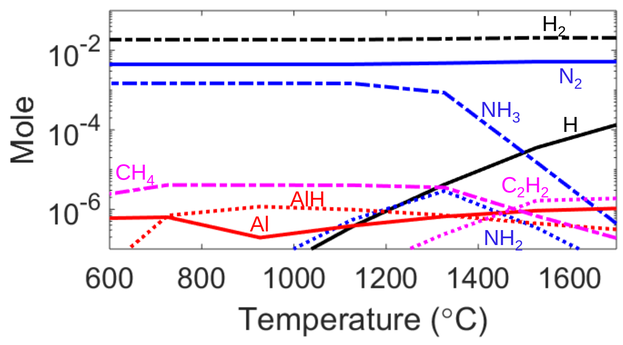
- 202 gas phase reactions (25 N-H, 1 H-H, 21 Al-(C)-H, 155 C-H reactions) and 46 species (14 Al-(C)-H species, 8 N-(H) species, 22 C-(H) species, H_2 and H atoms).

Input concentration: 18.6 mmole/sec H_2, 1.5 mmol/sec NH_3, 4.5 mmol/sec N_2, and 1.4 µmol/sec TMA

Thermodynamic equilibrium

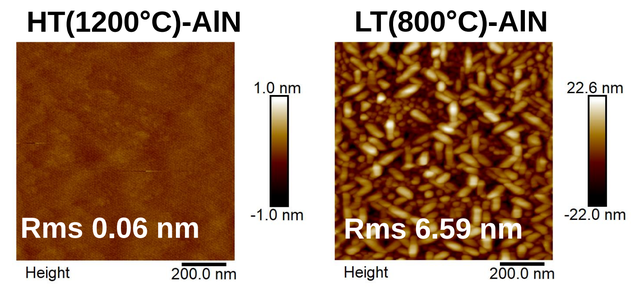


Kinetics, t_{kin} = 2 seconds



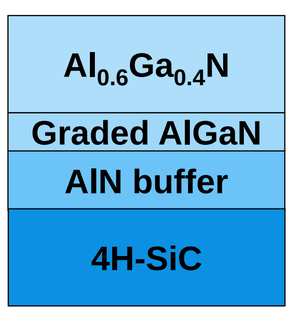
- Thermodynamics is applicable for Al- and C-species at T > 900 °C.
- Thermodynamics does not hold for N-species as it predicts that NH_3 changes into N_2. But this is too slow to occur noticeably for T < 1300 °C
- The most abundant species are Al and AlH for Al-species; NH_3 and NH_2 for N-species and CH_4 and C_2H_2 for C-species.

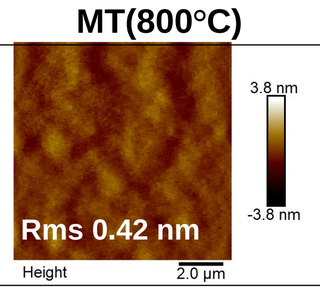
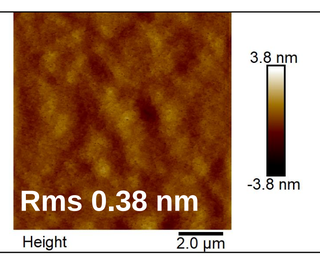
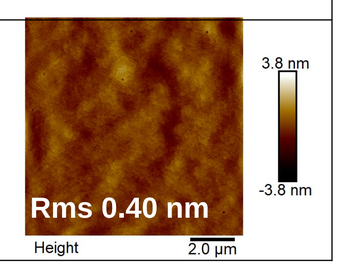
Effects of AlN growth mode



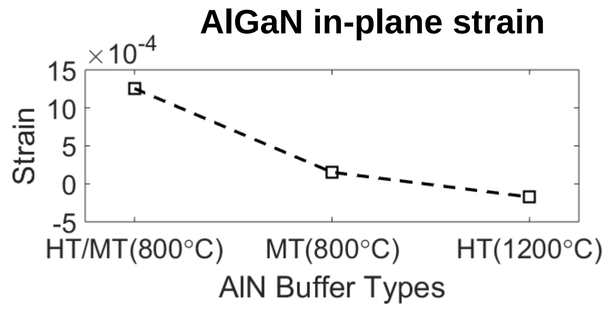
- AlN growth occurs in step-flow mode under HT condition, and island mode under LT condition.
- LT condition is used as a starting condition for multi-temperature (MT) growth before slowly being adjusted to resume step-flow growth.

Effects of AlN buffer types on AlGaN quality and strain

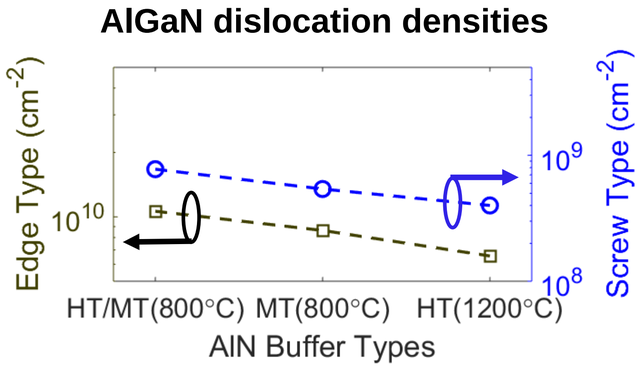


Buffers	HT(1200°C) on MT(800°C)	MT(800°C)-AlN	HT(1200°C)-AlN
AlGaN surface			

AlGaN in-plane strain

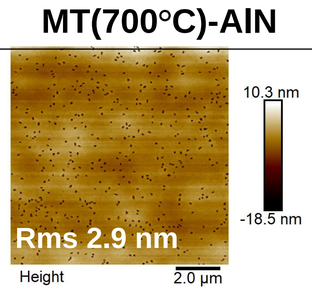
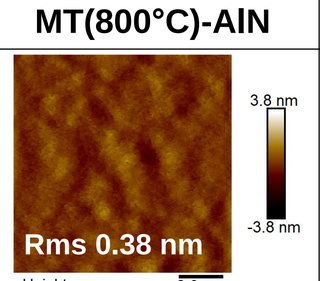
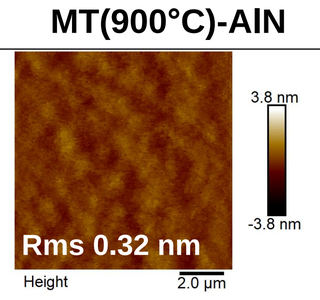
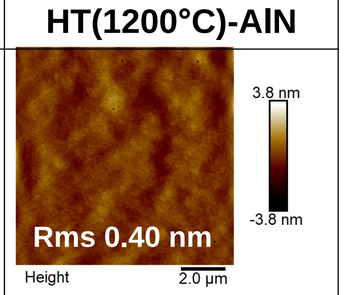


AlGaN dislocation densities

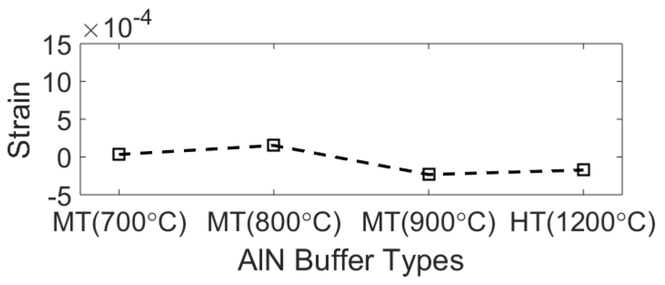


Compared to HT, AlGaN on MT buffers show similar morphology but higher strains and dislocations.

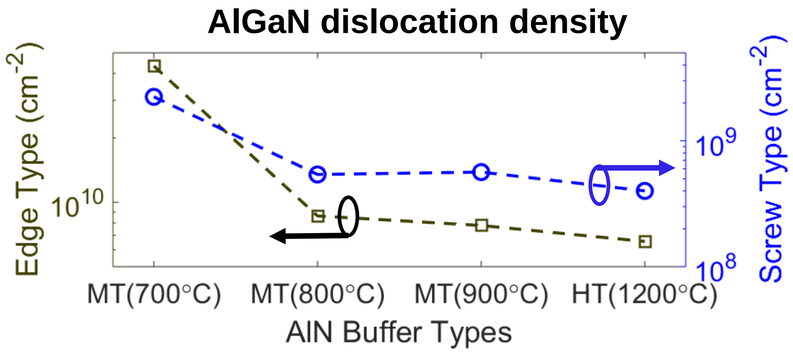
Effects of AlN buffer temperatures on AlGaN quality and strain

Buffers	MT(700°C)-AlN	MT(800°C)-AlN	MT(900°C)-AlN	HT(1200°C)-AlN
AlGaN surface				

AlGaN in-plane strain



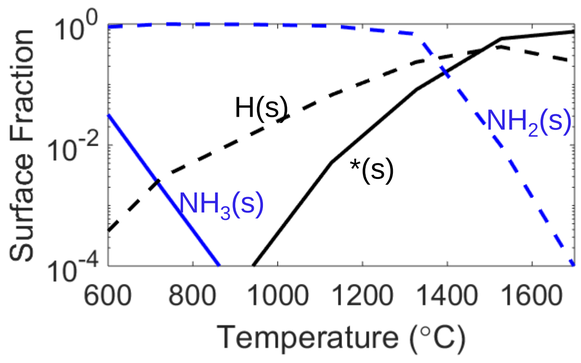
AlGaN dislocation density



- When MT temperature is lower than 800 °C, the AlGaN dislocation densities and surface quality deteriorate due to prolonged island growth mode.

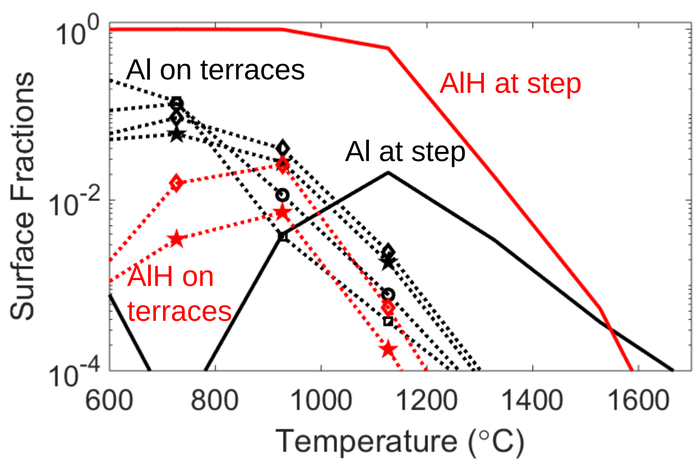
Growth model for AlN CVD

During NH_3-pretreatment[1]
Kinetic model at t = 3 seconds



- During the NH_3-pretreatment, the AlN terraces are mainly covered by NH_2(s) groups for T < 1300 °C.
- For T > 1300 °C, NH_2(s) groups become unstable and are replaced by hydrogen groups, H(s), and dangling bonds, *(s).

AlN growth[1]
Kinetic model at t = 3 seconds
Al and AlH as the main growth species.

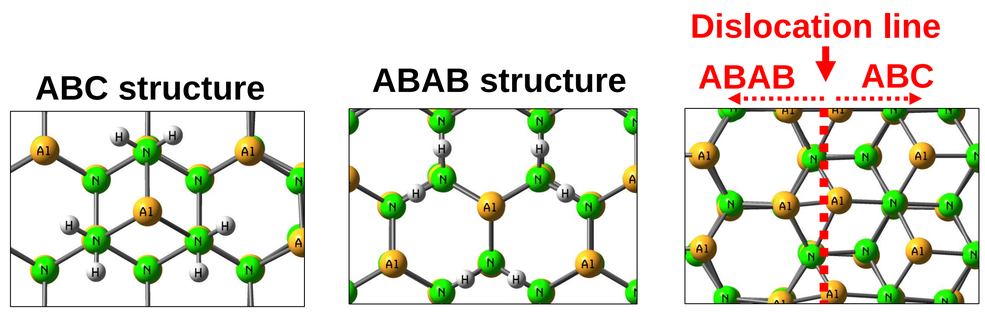


Black and red lines refer to Al and AlH groups. Marker types refer to adsorption sites:

"square" for NH_2(s), "circle" for 2 NH_2(s), "diamond" for 3 NH_2(s) as ABAB, "pentagram" for 3 NH_2(s) as ABC, and "no marker" for steps.

[1] DFT calculations were studied using $Al_{32}N_{32}$ and $Al_{39}N_{42}$ clusters at the theoretical level of B3LYP/SDD with Grimme D3 dispersion and electronic energy correction at B3LYP/cc-pVTZ.

Growth mode influence on dislocation formation



- Island growth produces dislocations along the boundaries where ABAB and ABC structures meet.
- Hence, it is *not only* the diffusion length but also the adsorption-site preference that determine the growth modes during the growth.
  - Al and AlH adsorptions on terraces (island growth) are significantly favored below 1000 °C (from ~1% occurrence at 1000 °C to > 20% at 600 °C).
  - Above 1000 °C, adsorptions become more favorable near step edges (step flow growth).

C3NiT - Janzén

LINKÖPING UNIVERSITY