Control of growth mode, dislocations and strain in Al-rich AlGaN by hot-wall MOCVD

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Challenges in the growth of Al-rich AlGaN

Heteroepitaxy of AlGaN at low temperature (LT) produces a rough surface dominated by screw dislocations. Utilizing high growth temperature (HT) and increasing AlGaN thickness can improve the quality and roughness, while also increasing the strain which may lead to crack formation during cooling down. Our strategy for improving the AlGaN is by controlling the growth mode of AlN buffer layers.

Method: Kinetic model of AlN CVD

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).

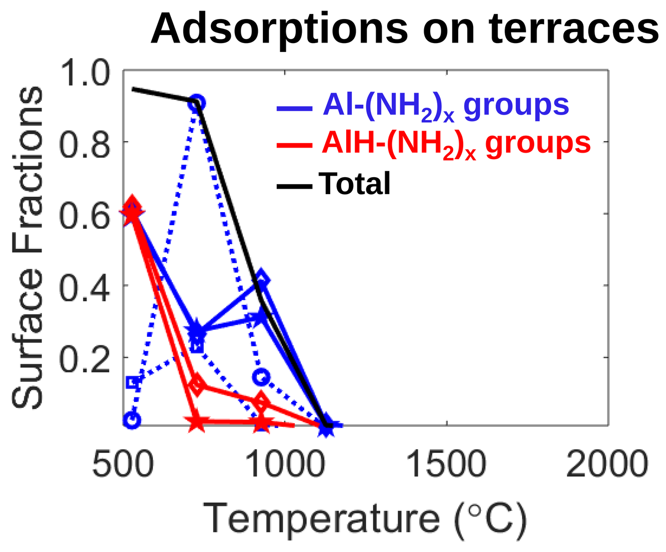
Surface kinetic model contains

- 27 surface reactions on terraces for 13 surface species.
- 20 surface reactions at step edges for 11 surface species.

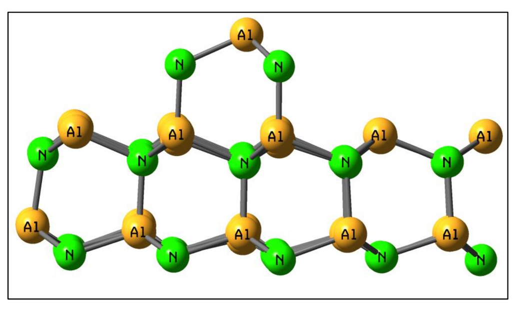
DFT calculations were performed using $Al_{32}N_{32}$ and $Al_{39}N_{42}$ clusters at B3LYP/SDD level with Grimme D3 dispersion and electronic energy correction at B3LYP/cc-pVTZ.

AlN growth on terraces (island growth)

Adsorptions on terraces occurs for T < 1100 °C.



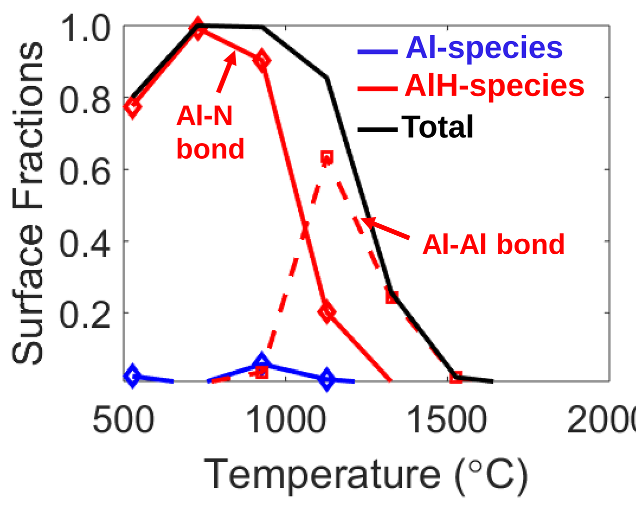
Input: 18.6 mmole/sec H_2, 1.5 mmol/sec NH_3, 4.5 mmol/sec N_2, and 1.4 µmol/sec TMA



Adsorption on terraces increases from 1% at 1100 °C to 90% at 700 °C.

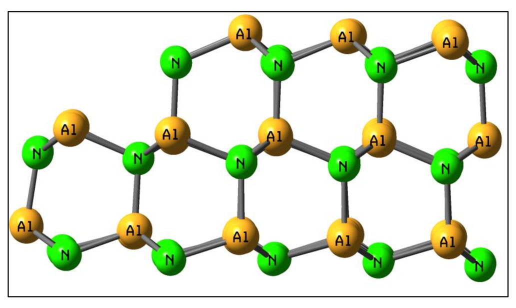
AlN growth at step edges (step-flow growth)

Growth at step edges is favorable for all temperatures.

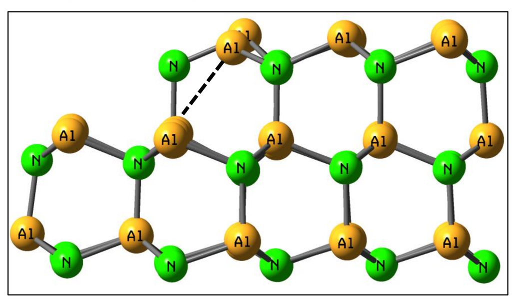


Input: the same condition as on terraces

Step-flow growth: Al-N bond



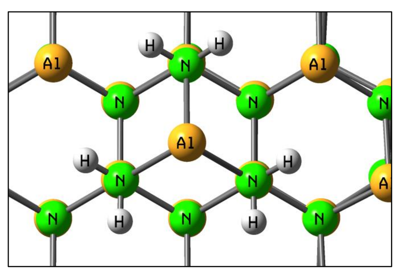
Step-flow growth: Al-Al bond



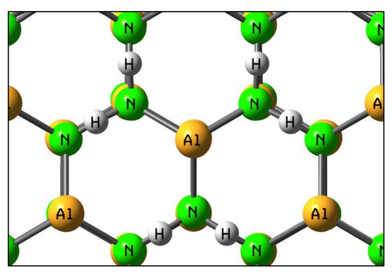
Al-N and Al-Al bond formations are favorable at T < 1100 °C and T > 1100 °C, respectively.

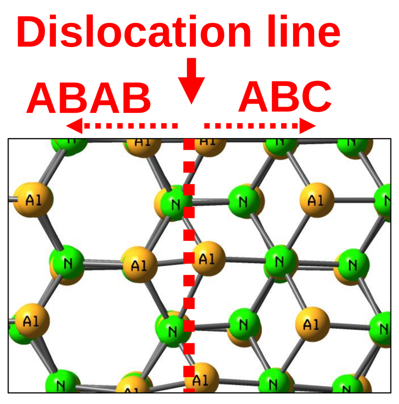
Growth mode influence on dislocation formation

ABC structure



ABAB structure



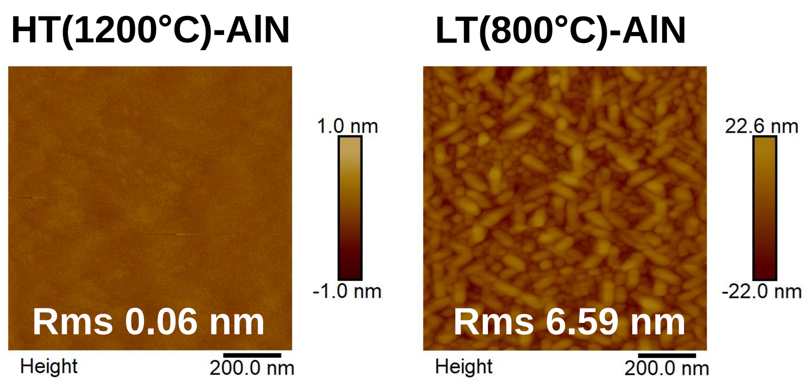


Island growth produces dislocations along the boundaries where ABAB and ABC structures meet.

Summary

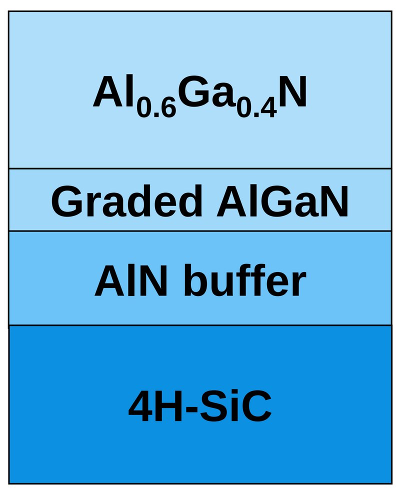
- We show experimental results on the effects of AlN buffer layers on the strain and dislocation densities in AlGaN layers.
- We present a CVD kinetic model of AlN which directly links the dislocation densities to the AlN growth temperature, and enables predictive growth strategies to reduce the dislocation densities.

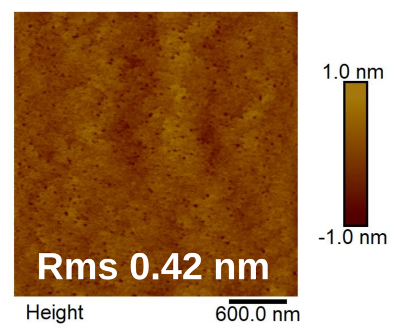
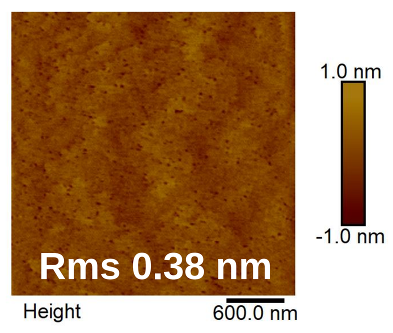
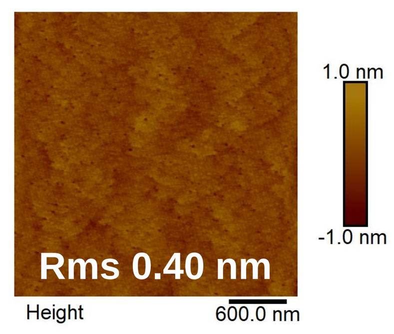
Effects of temperature on the growth mode of AlN buffer layers

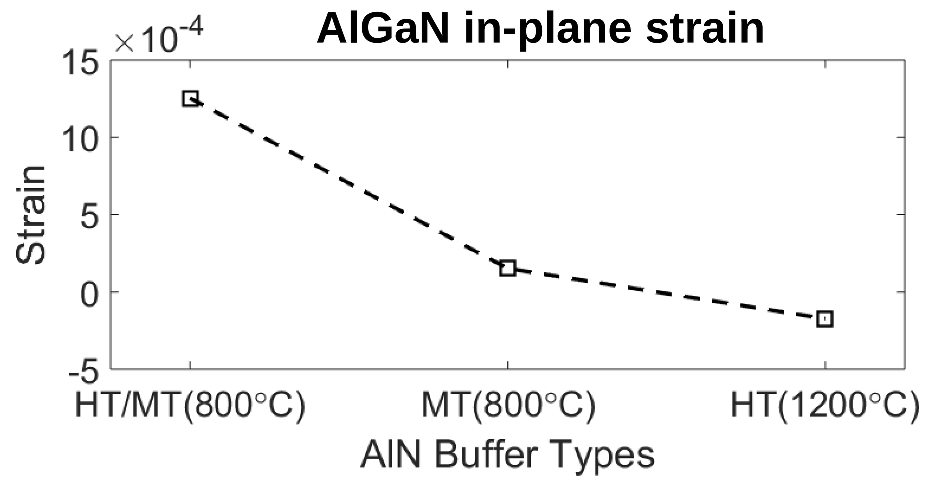


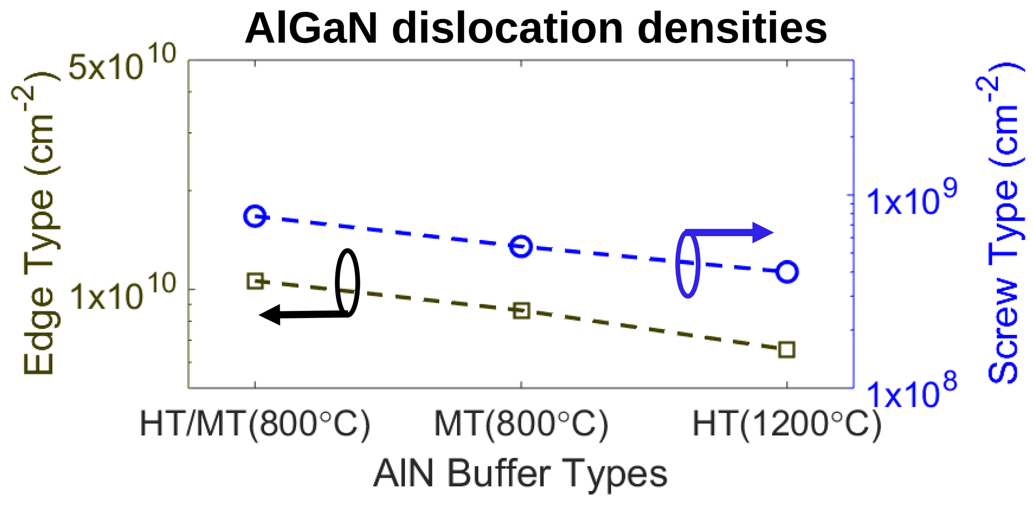
- AlN growth occurs in step-flow mode under HT condition and in island mode under LT condition.
- LT condition is used as a starting condition for multi-temperature (MT) growth before slowly being adjusted to resume step-flow growth.

Effects of AlN buffer types on AlGaN quality and strain



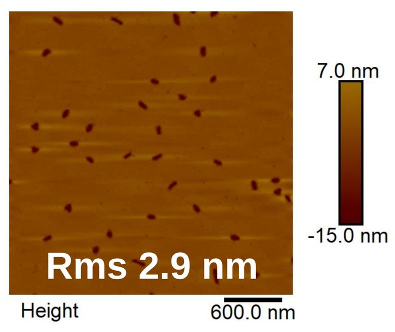
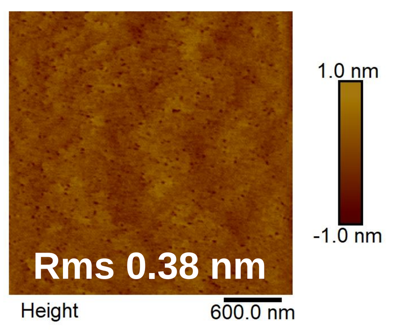
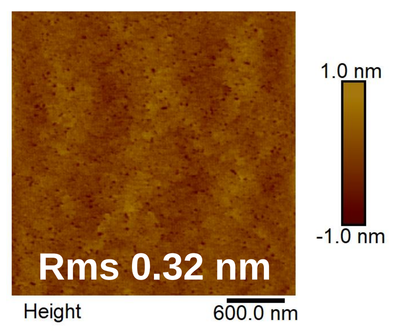
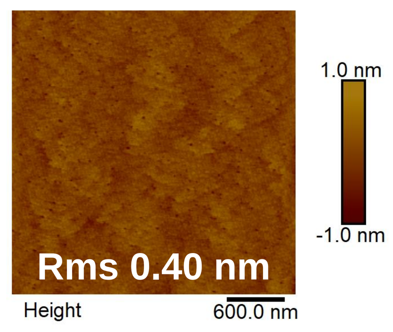
Buffers	HT(1200°C) on MT(800°C)	MT(800°C)-AlN	HT(1200°C)-AlN
AlGaN surface	 Rms 0.42 nm	 Rms 0.38 nm	 Rms 0.40 nm

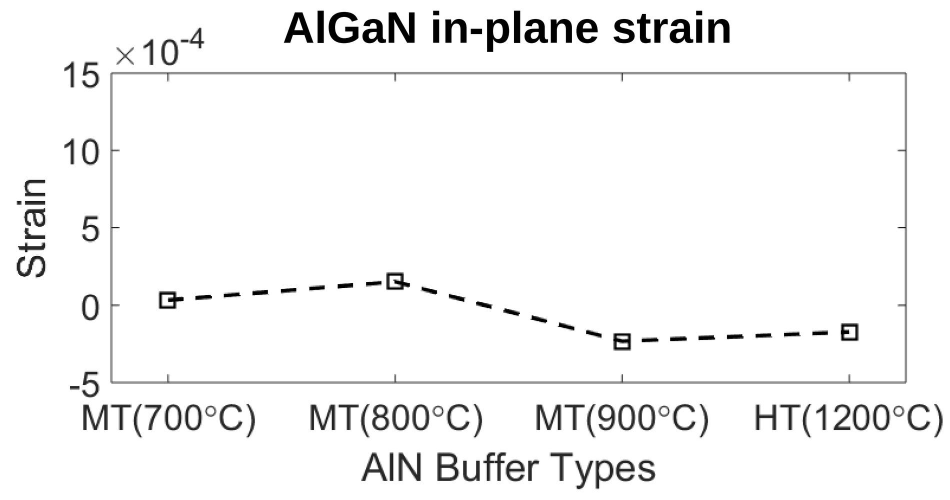


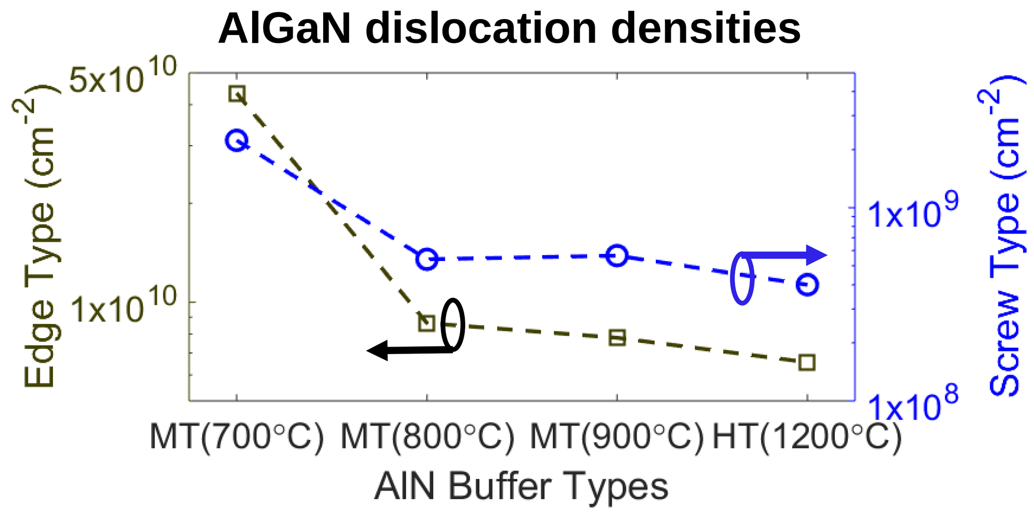


- AlGaN layers grown on MT, HT/MT and HT buffer layers show similar surface morphologies and dislocation densities.
- The in-plane strain of AlGaN layer grown on HT/MT(800 °C) increases significantly due to a high strain in the AlN buffer layer caused by a much larger temperature gradient during its growth.

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	 Rms 2.9 nm	 Rms 0.38 nm	 Rms 0.32 nm	 Rms 0.40 nm

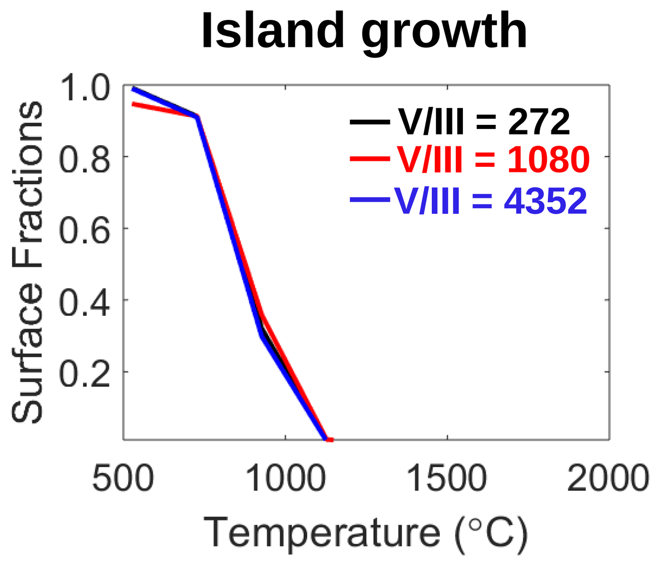




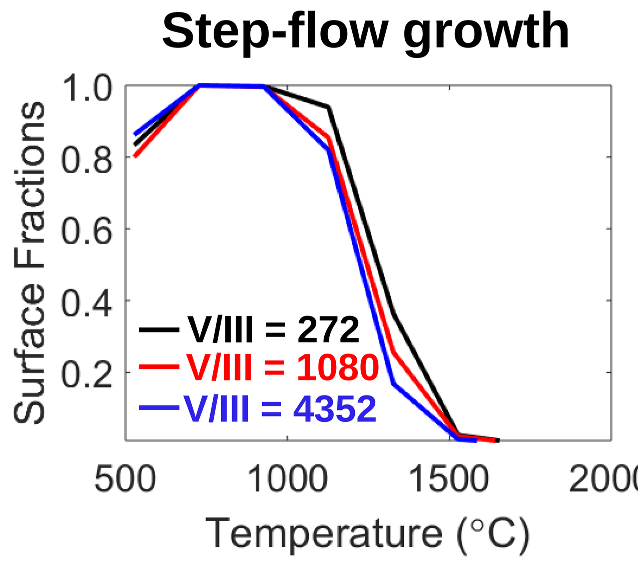
- MT with temperatures from 700 to 900 °C shows similar strains to the HT buffer.
- When T < 800 °C, the AlGaN crystal quality and surface deteriorate due to prolonged island growth mode. This indicates an insufficient recovery of the AlN buffer quality.

Model predictions

Island growth



Step-flow growth



The model predicts that:

- Increasing temperature is most effective in reducing dislocations in agreement with literature. [1]
- V/III ratios have little effect on island growth.
- Lowering V/III at T > 1000 °C increases the growth rate because Al-Al bond formation is favorable, in contrast to previous belief. [2]

1) S. Wang et al., Optik 126 (2015) 3698–3702.
2) M. Imura et al, J. Cryst. Growth 310 (2008) 2308-2313, Jpn. J. Appl. Phys. 45 (2006), 8639 and J. Cryst. Growth 300 (2007) 136-140.