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

Heteropolarity 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:

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 Al₂N₂ and Al₂N₃2 clusters at B3LYP/SDD level with Grimme D3 dispersion and electronic energy correction at B3LYP/cc-pVTZ.

A1N growth on terraces (island growth)

Adsorptions on terraces occurs for T < 1100 °C.

Input: 18.6 mmol/sec N₂, 1.5 mmol/sec NH₃, 4.5 mmol/sec N₂H₃, and 1.4 mmol/sec TMAl

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

A1N growth at step edges (step-flow growth)

Growth at step edges is favorable for all temperatures.

Input: the same condition as on terraces

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

- 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

- 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

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

References: