Hybrid NH_3/N_2 Molecular Beam Epitaxy with Artificial-Intelligence-Assisted Reflection High-Energy Electron Diffraction Analysis

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Abstract

Among various III-N epi growth methods, the hybrid molecular beam epitaxy (MBE) method can achieve good productivity for III-N epiwafers because it can produce an interface with excellent properties and afford a high growth rate. Furthermore, reflection high-energy electron diffraction (RHEED) analysis can be used for real-time measurements during MBE growth to obtain crystal structure information with atomic-level resolution. The crystal structure information is directly correlated to the epilayer quality and can thus be used to predict this quality. Automated RHEED analysis will be required to monitor the quality of a gallium nitride (GaN) high-electron-mobility transistor (HEMT) structure created by stacking tens of thousands of atomic layers. Toward this end, this study introduces an automated RHEED data prediction and analysis technique that employs a deep-learning-based artificial intelligence system. The results obtained by applying a machine-learning model to RHEED data for predicting the GaN HEMT quality are presented.

INTRODUCTION

Molecular beam epitaxy (MBE) grown III-N has been used in high performance high electron mobility transistors (HEMTs) for radio frequency (RF) applications.[1–4] With recent developments in regrown n^+ ohmic contacts, higher Al content (including binary) structures have been used in HEMTs and ultraviolet light-emitting diodes (UVLEDs);[4–6] this has resulted in increased interest in the use of MBE in such material systems. III-N MBE epi growth with N_2 plasma has been proven to be excellent for producing high-quality epi materials with abrupt interface control. However, N_2 plasma affords a limited growth rate compared with other techniques. To overcome this limitation for gallium nitride (GaN) MBE, IVWorks has developed a hybrid III-N MBE growth process that uses both N_2 plasma and ammonia sources. In this process, the N_2 plasma is applied for critical layers and the ammonia source affords a higher growth rate for thicker bulk layers.

Normally, reflection high-energy electron diffraction (RHEED) cannot be used for monitoring the entire MBE growth process of As, P, or Sb owing to the RHEED screen coating. Because As, P, or Sb exists as a solid at room temperature, it can be condensed and coated on RHEED screen that are cooler than ambient. Fortunately, in the III-N material system, N exists as a gas at room temperature, so there is no screen coating. In particular, RHEED can be applied to monitor and capture the entire GaN MBE growth process history for analysis and process control. In this light, the present study uses a novel artificial intelligence (AI)-assisted technique for analyzing RHEED patterns during MBE growth.

OVERVIEW OF DOMM™ AI EPITAXY SYSTEM

Domm™ is a patented AI technology that applies deep-learning algorithms for the detection and classification of RHEED patterns in an entire epi growth process. Specifically, a machine-learning model is used to analyze the collected

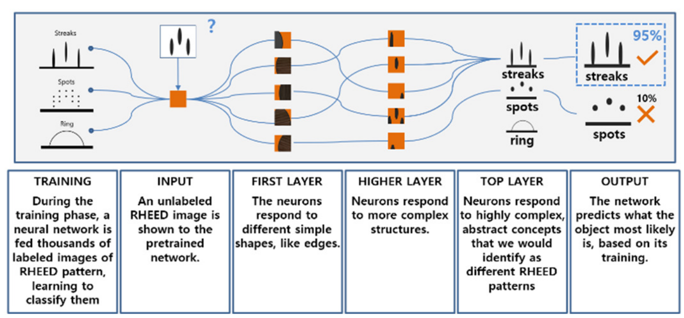

Fig. 1. RHEED pattern recognition by deep-learning based AI Epitaxy System, Domm™

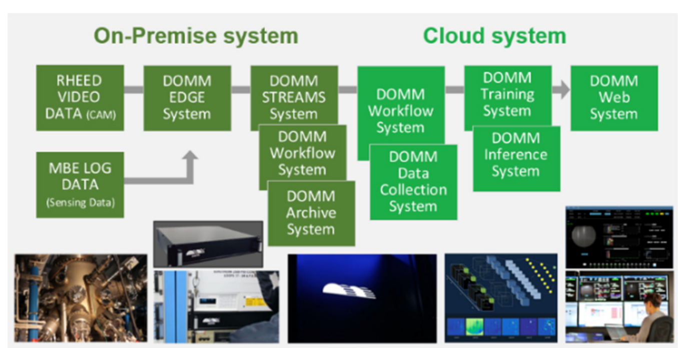

Fig. 2. Architecture of AI Epitaxy System, Domm™

data, such as the diffraction patterns throughout the entire structure, pattern transitions according to the growth mode and growth conditions, and equipment status. The correlations among the RHEED patterns, growth conditions, and final epiwafer quality are fed back to train Domm™ to create prediction models. This enables Domm™ to predict the quality of the growth process in real time before it is completed. Such information can be used to recommend recipe corrections to engineers when the predicted process quality is less than desired or to eventually correct a recipe autonomously to maximize productivity.

PREDICTION OF SILICON SUBSTRATE DEOXIDATION

In a heteroepitaxial system such as GaN on Si or SiC, the surface condition of the substrate and the deoxidation process are important steps in determining the epiwafer quality. For GaN grown on Si by MBE, the thermal deoxidation temperature of Si(111) is 700°C, and the RHEED pattern is

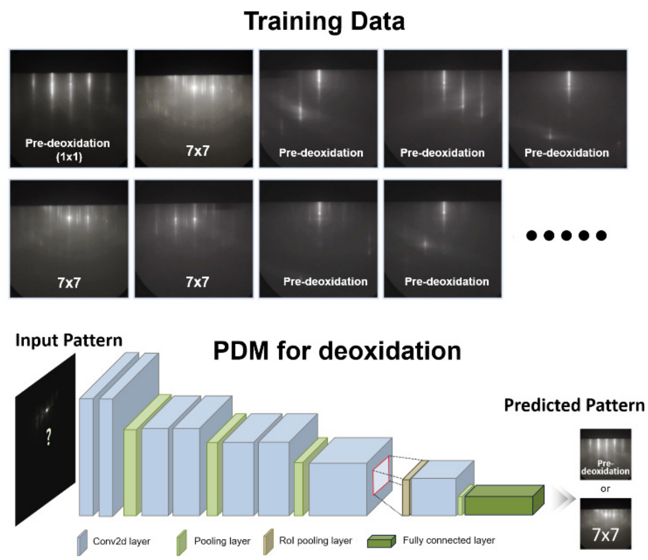

Fig. 3. Neural network architecture of PDM for deoxidation

known to change from 1×1 to 7×7.

Fig. 3 shows the training data and neural network architecture of a deep-learning-based pattern detection model (PDM) that was trained with various RHEED patterns of the Si(111) deoxidation process. The trained PDM could then detect RHEED patterns measured in real time during the deoxidation process and classify them by quantifying their probability-based similarity.

Fig. 4 shows the probability of achieving a 7×7 RHEED pattern during the deoxidation process using the PDM in Domm™. For a normal deoxidation process, the PDM predicts pre-deoxidation with almost 100% probability for all input RHEED images at a substrate temperature below 520°C. At higher substrate temperatures, the probability of predicting a 7×7 RHEED pattern increases rapidly; in particular, above 680°C, all input RHEED images are predicted as 7×7. By

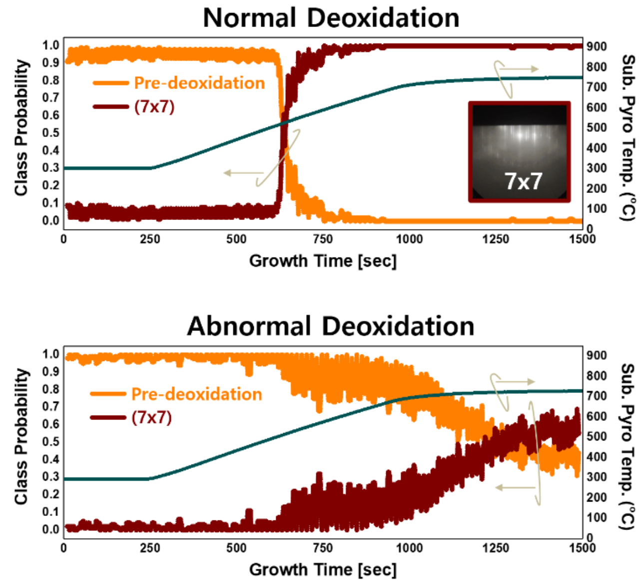

Fig. 4. Probability of achieving 7×7 RHEED pattern in two different runs

contrast, for an abnormal deoxidation process, the probability of predicting a 7×7 RHEED pattern decreases significantly with changes in the substrate temperature, indicating the occurrence of an abnormality.

PREDICTION OF ALGAN/GAN HEMT GROWTH

Fig. 5 shows the training data and neural network architecture of the PDM trained with RHEED patterns measured during the MBE growth of a GaN HEMT. In the MBE growth of III-N materials, the V/III ratio affects the

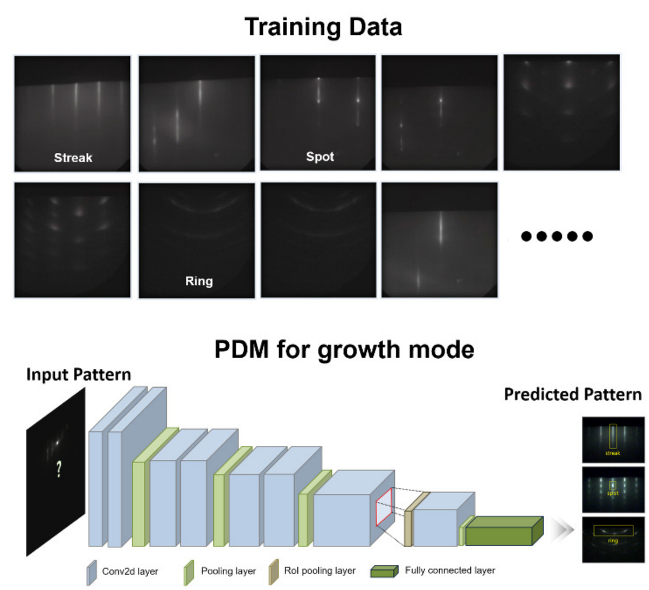

Fig. 5. Neural network architecture of PDM for growth mode

growth mode, and changes in the growth mode can be monitored through the RHEED patterns. When the RHEED pattern is a streak and a spot, the growth mode is 2D and 3D single crystalline, respectively.

Fig. 6a and 6b show the results of using the PDM to monitor the changes in the RHEED patterns when the NH_3 flow rate for the i-AlGaN buffer layer during the growth of a GaN HEMT was 760 and 460 sccm, respectively. The RHEED pattern was predicted using a PDM (Fig. 5) trained by inputting real-time RHEED patterns of the growth mode for the complete growth process of a 2.5 µm GaN HEMT structure. For the NH_3 flow rate of 760 sccm (Fig. 6a), the input RHEED patterns for the i-AlGaN buffer layer (3-4 region) were predicted as streaks with almost 100% probability. An atomic force microscopy (AFM) morphological analysis of the grown GaN HEMT epiwafer confirmed the step flow growth mode. By contrast, for the NH_3 flow rate of 460 sccm (Fig. 6b), the growth was less than ideal. The RHEED patterns look good during the first half of the growth process; this agrees with the prediction of streak patterns using Domm™. However, before time stamp 3', Domm™ sensed subtle changes and predicted a deteriorated surface. The result was indeed a spot RHEED pattern, and AFM revealed a high roughness.

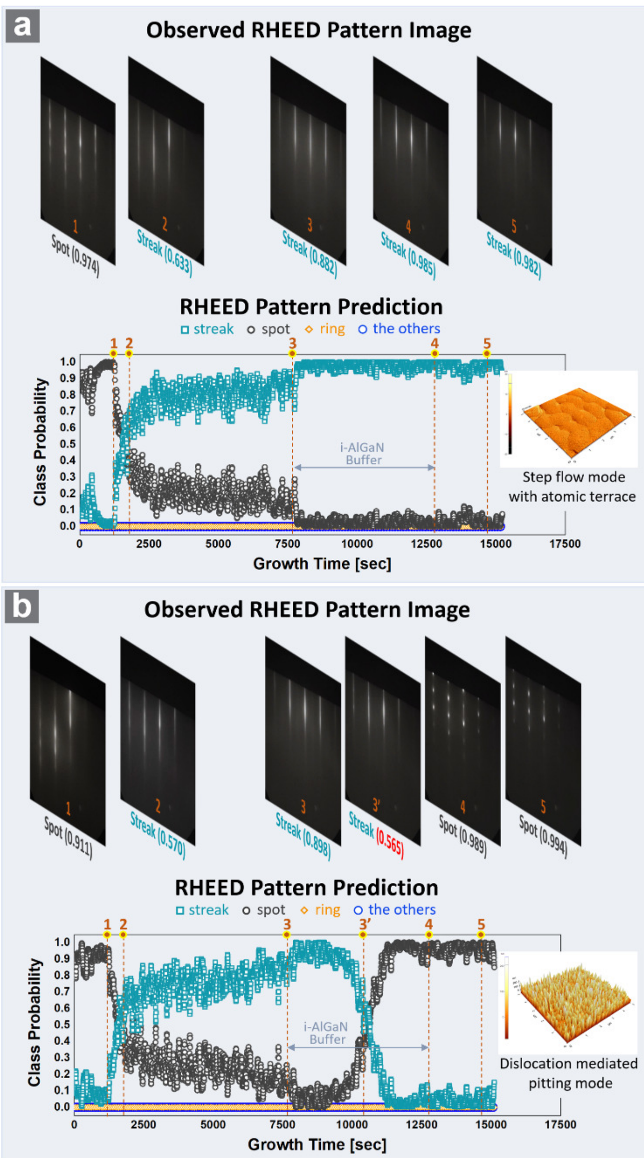

Fig. 6. Evolution of RHEED patterns during HEMT growth with NH_3 flow rates of (a) 760 sccm and (b) 460 sccm in i-AlGaN buffer

This demonstration clearly shows that the AI-assisted RHEED technique can be used to monitor and predict an epilayer surface before an engineer could detect its deterioration. The engineer can then adjust the growth condition or abort the growth process to minimize the loss of time and resources.

PREDICTION OF CRYSTAL QUALITY

RHEED can be used for real-time measurement and analysis of an MBE-grown epilayer surface to provide its crystal structure information with atomic-level resolution. Because the crystal structure information directly influences the epilayer quality, the quality can be predicted by analyzing the real-time RHEED data. Fig. 7 shows the training data and neural network architecture of the crystalline-quality prediction model (CPM) for predicting the X-ray diffraction (XRD) full width at half maximum (FWHM) (102), which

Training Data Set	• RHEED intensity • Class probability of PDM for deoxidation • Class probability of PDM for growth mode • Growth condition and sensing data • XRD FWHM (102)

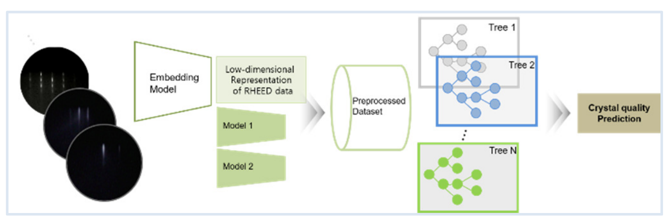

Fig. 7. Neural network architecture and training data of CPM

indicates the crystallinity of the GaN HEMT structure.

The CPM was trained using the RHEED intensity, PDM data, growth conditions, and MBE sensing data that were automatically collected using Domm™ during the growth of GaN HEMTs. It was also trained using the XRD FWHM (102) collected through measurements after the completion of the growth process. Fig. 8 shows a 2D vector space representation of the CPM prediction results for approximately 20,000 cases. Low and high (high and low quality) XRD FWHM (102) values, which indicate crystallinity, are indicated in gray and

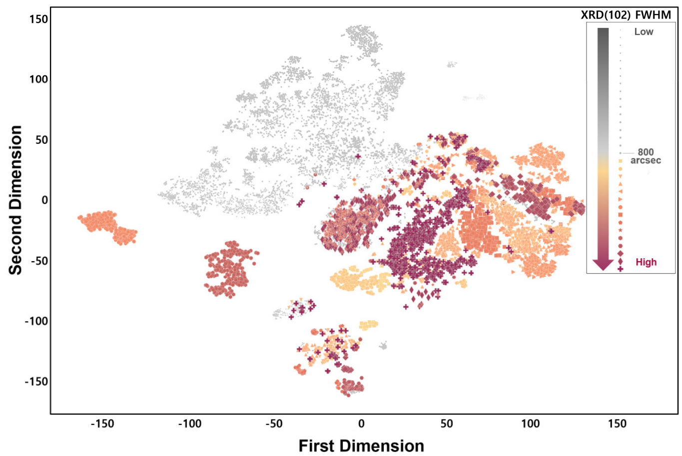

Fig. 8. Prediction result of CPM trained using dataset shown in Fig. 7

red, respectively. The gray values, indicating high quality with an FWHM of 800 arcsec or lower, were seen to be mostly grouped. This suggests that the CPM trained using the dataset shown in Fig. 7 provides excellent FWHM prediction results. Specifically, the CPM provided a high accuracy of 81.7%, precision of 74.1%, recall of 99.3%, F1 score of 84.8%, and area under curve (AUC) of 81.1%.

Summary and Advanced Capabilities of Domm™

The Domm™ deep-learning-based AI system was used to autonomously analyze and predict the quality of MBE-grown GaN HEMTs using RHEED data. Specifically, a deep-learning-based PDM was used to analyze the deoxidation process and AlGaN buffer layer growth mode of the Si(111) substrate during GaN HEMT epi growth. Further, a CPM trained using the RHEED intensity, PDM results, MBE sensing data, and XRD FWHM (102), which indicates the crystal quality of the GaN HEMT epiwafer, verified the excellent quality of the prediction result. We are developing a sheet resistance prediction model that is trained using lattice space information obtained from RHEED patterns. We will apply this technique to key layers during GaAs MBE growth. The use of RHEED analysis for As/P/Sb MBE growth may be somewhat limited owing to concerns about the screen coating, and only critical layers are monitored.

IVWorks will continue developing Domm™ to realize fully autonomous MBE growth control. Once the AI-assisted technique detects deviations in the RHEED patterns, it will adjust the recipe in real time to ensure that desirable results are obtained. Currently, Domm™ can be applied to GaN/SiC and GaN/Si HEMTs, and RHEED video and material results are being collected to train Domm™ to predict multiple epiwafer parameters. We expect that the fully developed Domm™ will be able to reduce the cost and improve the yield of GaN MBE growth through its monitoring/predicting capabilities.

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Acronyms

MBE: Molecular Beam Epitaxy
RHEED: Reflection High-Energy Electron Diffraction
GaN: Gallium Nitride
HEMT: High Electron Mobility Transistor
AFM: Atomic Force Microscopy
AI: Artificial Intelligence
PDM: Pattern Detection Model
CPM: Crystalline-Quality Prediction Model