Artificial Intelligence Optimization of MOCVD Growth for 800 nm GaAs Edge-Emitting Lasers.

A Data-Driven Approach to Improving Epitaxial Quality, Uniformity, and Manufacturing Yield

---

Abstract

The production of high-performance 800 nm GaAs edge-emitting lasers requires precise control of epitaxial layer thickness, alloy composition, dopant incorporation, interface quality, and wafer uniformity. Traditional MOCVD process optimization relies heavily on fixed recipes, statistical process control, and the experience of process engineers. However, reactor conditions evolve continuously throughout a production campaign as epitaxial material accumulates on internal reactor components, influencing temperature distribution, gas flow dynamics, precursor utilization, and ultimately device performance.

This paper proposes an Artificial Intelligence (AI)-driven Digital Twin that models the complete operational state of an MOCVD reactor throughout its production campaign. By integrating real-time process data, historical manufacturing information, physics-based growth models, and post-growth metrology, the Digital Twin continuously predicts epitaxial quality, reactor health, and remaining campaign life. A new concept, the Campaign State Index (CSI), is introduced as a latent process variable that characterizes the evolving condition of the reactor using cumulative deposited material, thermal history, morphology, photoluminescence stability, and other manufacturing metrics.

The proposed approach enables predictive process optimization, virtual recipe development, adaptive process control, and condition-based maintenance, allowing manufacturers to maximize wafer uniformity, improve repeatability, reduce process development time, and increase overall manufacturing yield for 800 nm GaAs edge-emitting laser production.

Introduction

Practical Digital Twin for an MOCVD Reactor

- A Digital Twin is far more than a three-dimensional model of an MOCVD reactor. It is a dynamic software representation that mirrors the physical reactor in real time by

combining live sensor data, historical process information, first-principles physics, and artificial intelligence. Every process variable measured during epitaxial growth continuously updates the virtual reactor, allowing it to predict wafer quality before the growth cycle is complete.

- For an 800 nm GaAs edge-emitting laser, the Digital Twin begins collecting information the moment a wafer cassette is loaded. The model identifies the substrate supplier, wafer orientation, off-cut angle, thickness, previous thermal history, and reactor maintenance status. It also records the complete operating history of the reactor, including the number of runs since the last chamber cleaning, showerhead replacement, graphite component replacement, and MFC calibration.
- During growth, the Digital Twin receives hundreds of data points every second from the reactor control system. These include reactor pressure, substrate temperature, susceptor rotation speed, TMGa, TMAl, arsine, and dopant gas flow rates, carrier gas composition, exhaust pressure, valve positions, and heater power. Rather than simply recording these parameters, the model evaluates how each variable interacts with every other process parameter.
- Using a combination of physics-based growth models and machine learning algorithms, the Digital Twin continuously predicts the growth rate, aluminum composition, layer thickness, quantum well dimensions, doping profiles, interface abruptness, and wafer uniformity. If the model detects that a critical parameter is beginning to drift outside its expected operating window, it can forecast the effect on the final laser performance before the wafer leaves the reactor.
- For example, a slight decrease in susceptor temperature may not immediately trigger an equipment alarm, yet the Digital Twin recognizes that this deviation could reduce aluminum incorporation, shift the quantum well emission wavelength, and increase threshold current. Instead of discovering the problem days later through photoluminescence or device testing, the system identifies the developing issue during growth and recommends corrective action.
- The Digital Twin also accumulates knowledge over thousands of production runs. Each completed wafer strengthens the predictive models by correlating growth conditions with post-growth measurements such as X-ray diffraction, photoluminescence, Hall measurements, AFM surface morphology, and final laser performance. As more production data become available, prediction accuracy steadily improves.
- Perhaps the greatest advantage of a Digital Twin is the ability to perform virtual experiments. Process engineers can evaluate changes in temperature, pressure, gas flow, or growth sequence within the virtual reactor before committing valuable production wafers. Hundreds of potential recipes can be simulated overnight, allowing only the most promising candidates to move into production trials. This dramatically shortens process development cycles while reducing material consumption and reactor time.
- Over time, the Digital Twin evolves from a monitoring tool into an intelligent process advisor. Rather than relying solely on fixed recipes developed through years of engineering experience, the reactor becomes a continuously learning manufacturing system capable of predicting process outcomes, recommending optimal operating conditions, and supporting real-time process optimization for consistent production of high-performance 800 nm GaAs edge-emitting laser structures.

Digital Twin: Modeling the MOCVD Campaign Lifecycle

While conventional Digital Twins focus primarily on equipment diagnostics, a practical Digital Twin for an MOCVD reactor must model the reactor's campaign lifecycle. The condition of the reactor evolves continuously as epitaxial material accumulates on the graphite susceptors, chamber walls, showerhead, and other internal components. These changes directly influence temperature distribution, gas flow dynamics, precursor depletion, and ultimately epitaxial quality.

The Digital Twin should recognize that every production campaign consists of three distinct operating phases.

Campaign Start – Reactor Stabilization

Immediately following a reactor clean and rebuild, the reactor is not yet in its optimum operating condition. The freshly exposed graphite surfaces and clean reactor geometry produce growth characteristics that differ significantly from those observed later in the campaign. During this stabilization period, several microns of epitaxial deposition are typically required before temperature distribution, precursor chemistry, and growth uniformity become repeatable. Experienced process engineers often refer to this as "seasoning" the reactor.

Rather than treating these initial wafers as isolated production runs, the Digital Twin tracks the cumulative deposited thickness throughout the campaign and predicts when the reactor has entered its stable operating window. Historical production data allow the model to estimate the number of deposited microns required to achieve target wafer-to-wafer repeatability and within-wafer uniformity for a specific reactor configuration.

Stable Production Window

Once the reactor has been sufficiently seasoned, it enters the most productive phase of the campaign. During this period, layer thickness, alloy composition, photoluminescence wavelength, and wafer uniformity remain well controlled. The Digital Twin continuously compares live process data against historical campaigns to verify that the reactor remains within this optimum operating window and provides early warning of subtle trends before they become measurable product deviations.

Campaign End – Predicting Performance Degradation

As additional material accumulates throughout the campaign, the reactor gradually departs from its optimum state. Deposition on internal reactor surfaces alters thermal characteristics and gas flow patterns, increasing the probability of process drift.

In practice, production campaigns generally end for one of two reasons:

1. Surface morphology degrades beyond acceptable limits, resulting in increased roughness or other crystal quality defects.
2. Alloy composition and photoluminescence wavelength can no longer be maintained within process specifications despite recipe adjustments.

The Digital Twin continuously correlates cumulative deposited thickness, reactor operating history, morphology measurements, X-ray diffraction, photoluminescence wavelength, and final device performance to estimate the remaining useful life of the campaign. Rather than relying on fixed cleaning intervals, the system predicts the optimum endpoint for each campaign based on actual reactor behavior.

This transforms reactor maintenance from a calendar-based activity into a predictive manufacturing strategy. Instead of asking, "How many runs have we completed?", engineers can ask, "How much useful campaign life remains before epitaxial quality begins to deteriorate?" By forecasting both the stabilization period at the beginning of a campaign and the degradation mechanisms at its end, the Digital Twin maximizes productive reactor time while maintaining consistent epitaxial quality for high-performance 800 nm GaAs edge-emitting laser structures.

While many Digital Twin implementations emphasize equipment diagnostics and sensor monitoring, the operating condition of an MOCVD reactor is more accurately characterized by its campaign state, which evolves continuously throughout the production cycle. AI should be learning the *evolution of the reactor* over the entire campaign, not just monitoring temperatures and gas flows.

Campaign State Index (CSI).

Problem Statement:

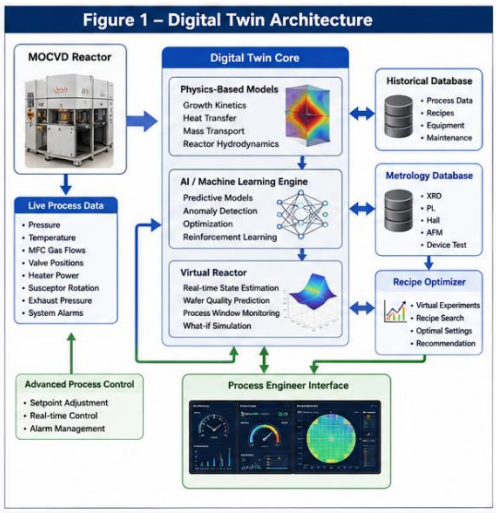
Every MOCVD reactor has an operating state that evolves continuously throughout a production campaign. This state cannot be measured directly by a single sensor. Instead, it must be inferred from the combined effects of cumulative epitaxial deposition, thermal history, reactor maintenance, gas flow characteristics, and measured epitaxial performance.

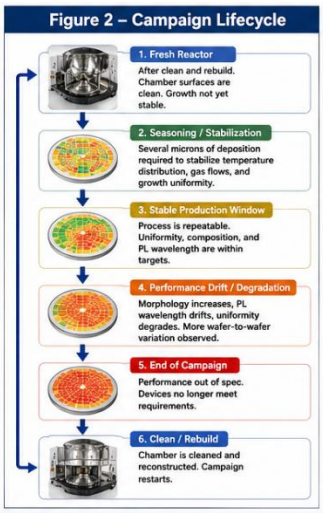
Rather than using *run count* or *days since PM*, the AI would estimate:

- **CSI = 0–20**: Fresh reactor (seasoning phase; uniformity not yet stabilized)
- **CSI = 20–85**: Stable production window
- **CSI = 85–100**: End-of-campaign; increasing risk of morphology degradation and photoluminescence wavelength drift

The CSI would be learned from historical data—not defined by a fixed number of runs. Inputs could include cumulative deposited microns, cumulative aluminum-containing growth, temperature trends, photoluminescence wavelength stability, thickness uniformity, morphology measurements, and reactor maintenance history. This approach reflects how experienced

MOCVD engineers actually judge reactor condition while giving AI a quantitative target to predict and optimize.





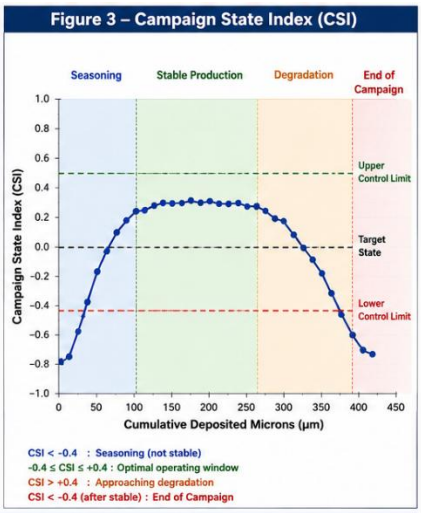


Table 1 – Campaign State Index (CSI) Inputs

Category	Input Parameter	Description	Source	Update Frequency
Process Conditions	• Reactor Pressure • Susceptor Temperature • MFC Gas Flows (TMGa, TMAl, AsH_3, Dopants) • Carrier Gas Composition • Exhaust Pressure • Susceptor Rotation Speed • Heater Power	Real-time operating conditions that directly affect growth kinetics, mass transport, and temperature distribution.	Reactor Control System (PLC / SCADA)	1–10 Hz (real time)
Cumulative History	• Cumulative Deposited Microns • Cumulative Al Deposition (mol/cm²) • Runs Since Last Clean • Component Age (Showerhead, Susceptor, etc.)	Represents the physical evolution of the reactor as material accumulates on internal surfaces.	Digital Twin (Calculated)	Per Wafer / Per Run
In-situ / Inline Indicators	• Growth Rate • In-situ Uniformity (optical / pyrometry) • Chamber Temperature Uniformity	Indicators of immediate process stability and uniformity.	In-situ Sensors / Pyrometry	1–10 Hz (real time)
Post-Growth Metrology	• Photoluminescence (Wavelength, FWHM, Intensity) • X-ray Diffraction (Al Composition, Strain) • Hall Measurements (Carrier Concentration, Mobility) • AFM Surface Morphology (RMS, Defect Density) • Device Test (Threshold Current, Slope Efficiency)	Direct measurements of epitaxial quality and device-relevant parameters.	Metrology Tools / Device Test	Per Wafer (after growth)
Equipment & Maintenance	• Maintenance Events • Alarm History • MFC Calibration History	Equipment condition and maintenance impact future process stability.	Manufacturing Execution System (MES)	Per Event / Per Run

Figure 1. Integrated Digital Twin Model for MOCVD Campaign Management

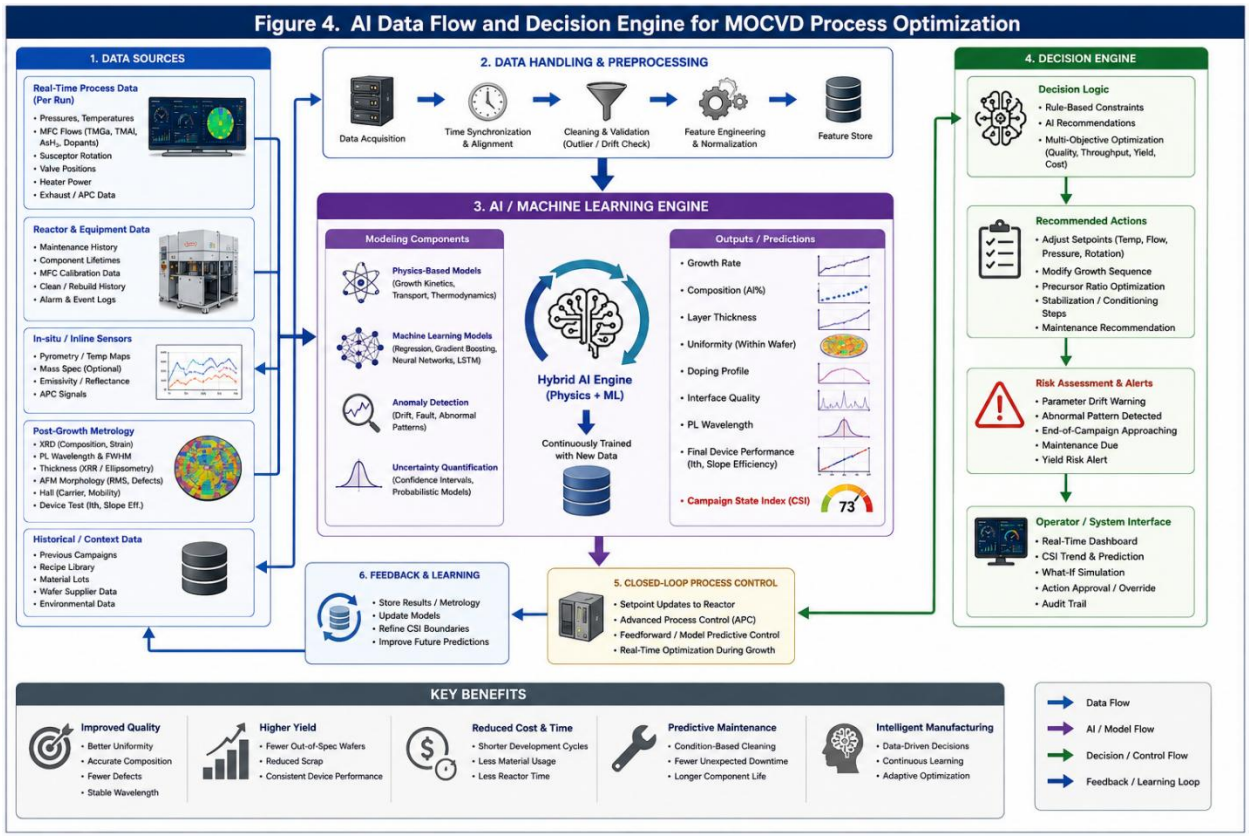


Figure2: AI Data Flow and Decision Engine for MOCVD Process Optimization

Conclusion

Artificial Intelligence has the potential to fundamentally change the way MOCVD reactors are operated for the production of 800 nm GaAs edge-emitting lasers. Rather than relying solely on fixed process recipes, statistical process control, and engineering experience, AI enables the creation of a continuously learning Digital Twin capable of modeling the complete operational state of the reactor throughout its production campaign.

The introduction of the **Campaign State Index (CSI)** provides a practical framework for quantifying reactor condition using cumulative deposition history, real-time process measurements, post-growth metrology, and historical manufacturing data. By continuously estimating the evolving campaign state, the Digital Twin can predict the onset

of morphology degradation, photoluminescence wavelength drift, and other process deviations before they impact production yield.

Beyond monitoring reactor performance, this approach enables predictive maintenance, virtual recipe development, adaptive process optimization, and data-driven manufacturing decisions. As additional production campaigns are completed, the Digital Twin continuously refines its predictive capability, allowing each reactor to develop an increasingly accurate understanding of its own operating characteristics.

Although this paper focuses on 800 nm GaAs edge-emitting lasers, the proposed methodology is broadly applicable to other III-V semiconductor devices, including VCSELs, high-power laser diodes, HEMTs, HBTs, and photonic integrated circuits. The combination of physics-based reactor modeling and artificial intelligence represents a significant step toward autonomous semiconductor manufacturing, where process optimization is driven not only by engineering expertise but also by continuously learning predictive models.