HPC4 MANUFACTURING

# Project Aims to Reduce Costs and Manufacturing Time for Next-Generation LEDs

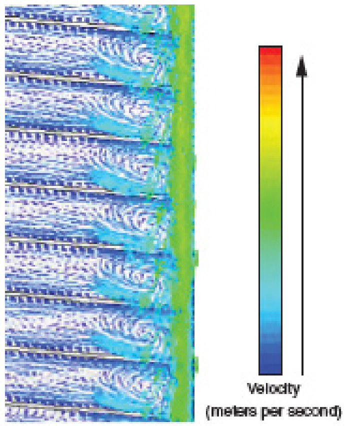
*Livermore is working with light-emitting-diode (LED) manufacturer SORAA to create a new computer model of the company's research-scale process for growing gallium nitride (GaN) crystals.*

## Looking to the Future of LEDs for New Applications

Gallium nitride (GaN) is an emerging semiconductor material making inroads in many technological areas. One application that most people are familiar with is the Blu-ray player, which uses a violet laser diode on a GaN substrate to read Blu-ray DVDs.

For GaN-based light-emitting diodes, GaN layers are typically deposited on a nonnative substrate, such as sapphire or silicon carbide, leading to lattice strain between the two materials that can reduce device reliability and performance. GaN-based devices that use a GaN substrate (known as GaN-on-GaN technology) have higher power operation and higher efficiencies than those made with traditional semiconductor materials. As a result, they also have the potential to drastically cut energy consumption in consumer applications. The challenge to making GaN-on-GaN devices for commercial products is finding scalable ways to grow high-quality crystals of the material quickly and inexpensively.

Through a project funded by the Department of Energy's High Performance Computing for Manufacturing (HPC4Mfg) program, which aims to provide supercomputing resources to industry partners, Lawrence Livermore National Laboratory is working with LED manufacturer SORAA to create a new computer model of the company's research-scale process for growing GaN crystals. The goal of the effort is to help improve the crystal-growth process, leading to widespread adoption of GaN for




Laboratory simulations of the SORAA reactor showed more turbulent gas flow than previously anticipated.

substrates in solid state lighting and power electronics, among other applications.

## Scaling Up Industrial Processes Using High-Performance Computing

Semiconducting materials are typically grown using melt techniques. However, GaN crystals cannot be grown using such methods because GaN's melting temperature is exceedingly high (2,500 degrees

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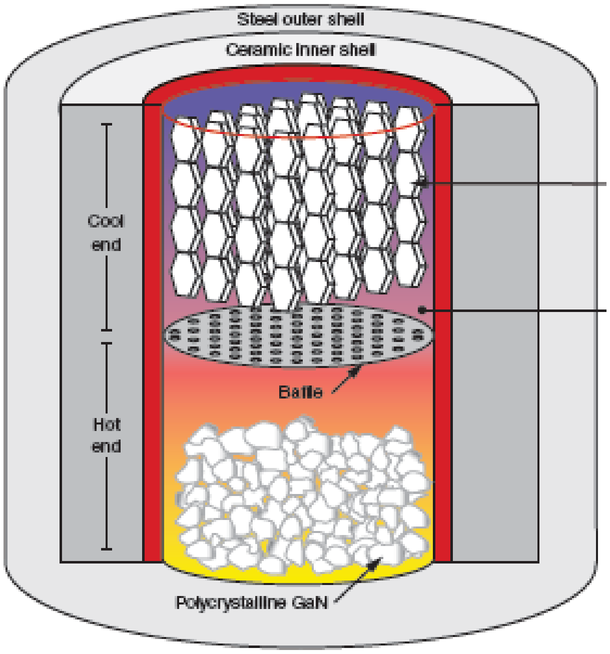
Celsius), and high pressures are needed to keep the material from decomposing into its two elemental constituents. The most common GaN production process is hydride vaporphase epitaxy (HVPE), which involves reacting ammonia with gallium chloride at about 1,100 degrees Celsius. Although this process has high growth rates, it is also expensive and usually results in crystals with too many defects for many applications.

SORAA, a Fremont, California-based company, was co-founded by Nobel Prize–winning physicist and University of California at Santa Barbara professor Shuji Nakamura, who invented the first high brightness LED. The company builds LED lamps using GaN-on-GaN substrates and says the resulting high-powered violet LEDs are not only brighter and whiter than conventional LEDs, but are also safer because long-term exposure to blue light LEDs can can cause health problems. However, their research process for creating the single crystal GaN needed for a substrate is complicated and requires a sealed reactor, making it difficult for researchers to analyze the process. Furthermore, to increase production rates, new, larger reactors will be needed. Accurate modeling of the conditions in the reactors will enable scale up to higher volume apparatuses.

SORAA partnered with Livermore through the HPC4Mfg program to better understand the crystal growth processes inside the reactor using multiphysics simulations run on the Laboratory's high-performance computing systems. Previously, SORAA had run simulations on a 12-processor workstation, which limited what physics could be incorporated in their models and the number of cases that could be studied. Laboratory supercomputers were able to capture the complex physics processes in considerably less time. On the workstation, SORAA simulations took an entire week to complete. The Laboratory systems reduced the processing time by 10 fold.




Livermore supercomputers were used to simulate the physics processes occuring inside SORAA's reactor (shown here) for growing high-quality gallium-nitride (GaN) crystals.

## Higher Resolution Simulations Show Unsteady Gas Flow

The Livermore team used a licensed, commercial code to develop a computational fluid dynamics model that could simulate the high pressure and intense heat needed for the GaN growth process. The simulations, run on the Laboratory's powerful supercomputers, incorporate more mesh points, allowing researchers to better understand the gas flow within the reactor and track how the environment changes with time. Results from the higher fidelity simulations revealed a much more complicated flow structure than anticipated. Modeling the flow and temperature profile along the walls of the reactor showed a flow that was transient and turbulent. The results improved predictions of local temperatures and flow velocities, providing valuable insight.

SORAA is committed to further improving upon the Livermore models and evaluating various computationally developed reactor configurations to select the most promising designs. The best-performing ones will then be tested experimentally with the goal of producing large, production-scale reactors.

As a result of this collaboration, SORAA is now in a better position to optimize the uniform growth of GaN crystals. Once large crystals can be grown quickly and with fewer defects, the door will be open for wider use of GaN in high-power electronics and other applications.

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