Computational Study of Flow and Growth Inside Ammonothermal Gallium Nitride Reactor

CPS Agreement Number:29332

SORAA HPC for Manufacturing Project partnering with LLNL

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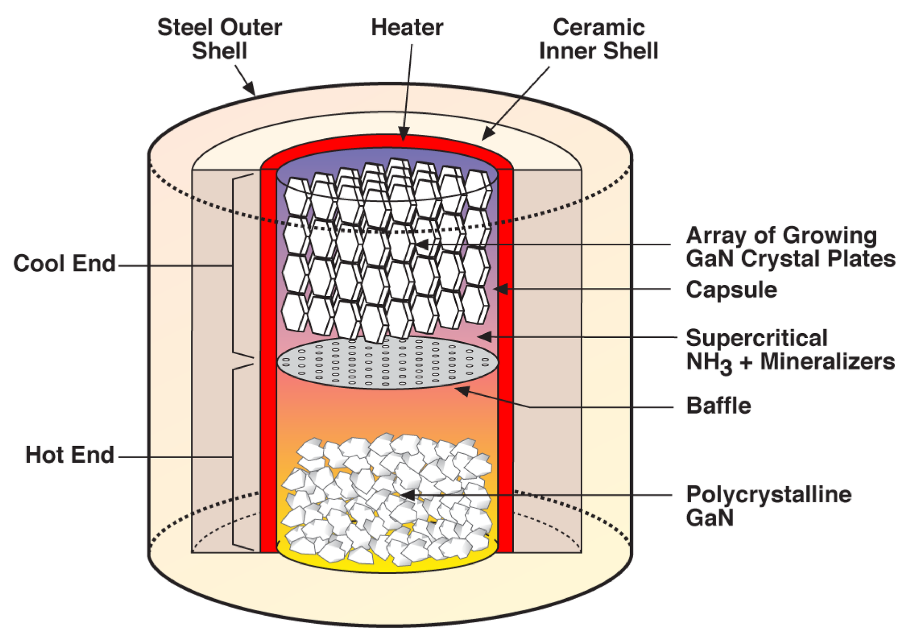
Project Objective

We use high performance computing (HPC) for multi-physics simulations to understand the growth of gallium nitride (GaN) during the ammonothermal process, which could significantly reduce the cost of LED lighting and spur the next generation power electronics.

- Current methods of producing gallium nitride (GaN) are too costly for use as a substrate for LED lights.
- The ammonothermal process is a promising new approach to synthesize single crystal GaN, but not well understood and difficult to analyze experimentally.

Working Principle of Ammonothermal Process



Temperature gradient in reactor induces buoyancy driven convection loop transporting GaN from nutrient region on the bottom to growth region on the top. Solubility decreases as solvent cools in cold upper region and GaN is deposited on GaN seeds.

Technical Innovation

SORAA has been conducting computational fluid dynamic simulations, but has limited computing resources restricting model fidelity and throughput.

HPC captures key physics otherwise missed using high-end workstations

- Higher mesh resolution and more complex turbulence models better capture temperature gradients at the wall and the transition to turbulent flow that affects the local crystal growth rate.
- Transient simulations show that the average fluid behavior is not captured in the steady-state solution.

Approach

We are combining Soraa's specialized crystal growth knowledge and LLNL's expertize in simulating reactive flows on HPC to better understand the flow physics affecting growth inside the ammonothermal reactor.

- Soraa provides reactor geometry, process conditions, baseline simulation setup, experimental data and one- of-a-kind knowledge of the process.
- LLNL provides unique expertise in setting up and running parallel reacting flow simulations and the compute resources to run them.
- A potential risk is that some properties of the ammonia solvent are unknown at the extreme conditions of this process. We will validate the simulations with experimental data and perform a sensitivity analysis to understand their impact on the results.

Transition and Deployment

Working together we have demonstrated the value of HPC in increasing our understanding of the ammonothermal process. Furthermore, LLNL is training Soraa to setup and run simulations on HPC resources to increase the industry impact.

- Soraa will use the knowledge it gains from simulations to improve its production of GaN, leading to lower cost LED lights and opening up new applications for GaN.

Measure of Success

- Insight gained from this project could reduce the cost of full spectrum LED lights thereby increasing the market adoption.
- EIA estimates that a large scale adoption of LED lights would reduce US electricity consumption by up to 20%.
- Low cost GaN will also have a large impact on laser diodes and high power electronics devices.

Project Management and Budget

1-year project with the following key milestones

- Demonstrate ability to simulate reactor and document best practices
- Validate model with chemistry using experimental growth rates

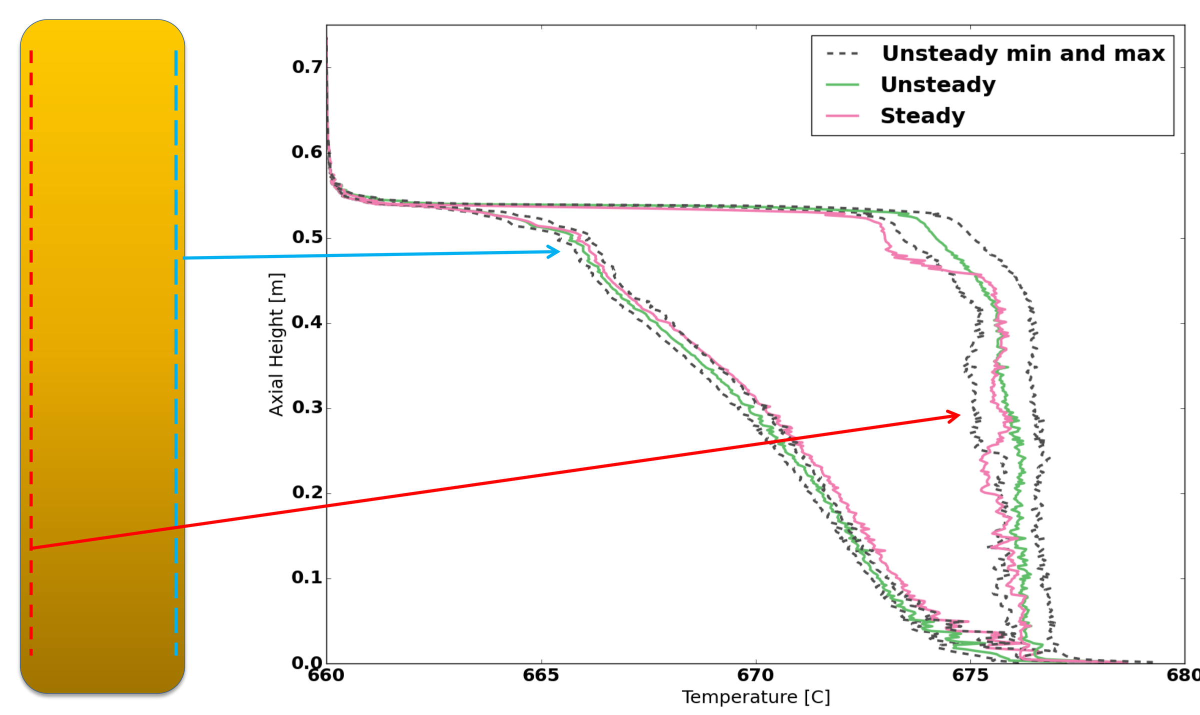
Total Project Budget	
DOE Investment	$310
Cost Share	$100k
Project Total	$410k

Results and Accomplishments

This project has achieved the following in the first 8 months:

- Performed dozens of solver studies to establish best practices for GaN reactor simulations
- Documented best practices to help industry users
- Demonstrated HPC increases throughput +10x
- Proved HPC necessary to capture key physics:
  - finer meshes for accurate temperature gradients near the growth sites
  - finer meshes for turbulent flow transition
  - unsteady solver to capture true mean

Demonstrated Flow is Unsteady



Time-dependent, full 3-dimensional simulations show that the temperature along two vertical lines in the reactor varies with time and that the average temperature at each height differs from the steady solution

We are currently adding chemistry to the model, which will allow direct comparison of growth rates to experimental data.

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