Computation Study of Flow and Growth Inside Ammonothermal Gallium Nitride Reactor

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SORAA

Rajeev Pakalapati (Soraa Inc.)

Nick Killingsworth (LLNL)

Lawrence Livermore National Laboratory

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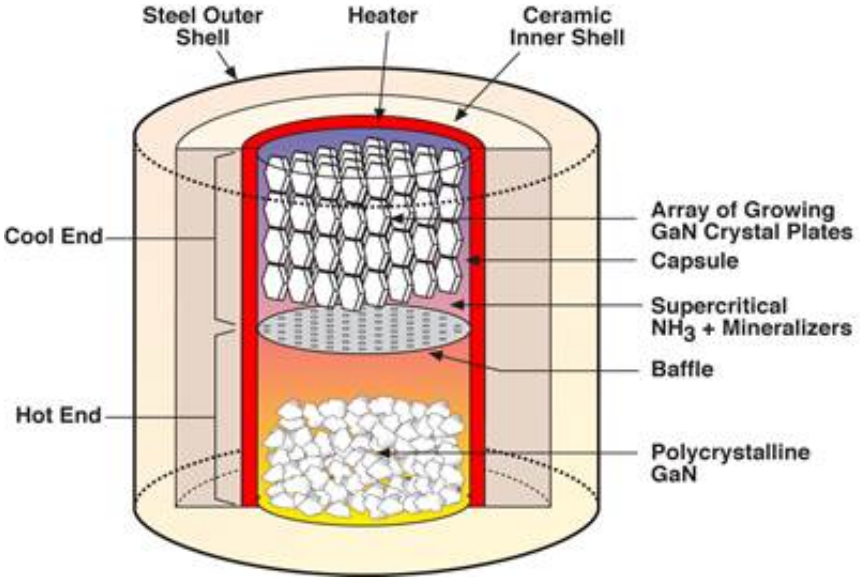
Project Objective

- Soraa is an LED-based lighting manufacturer and is the largest consumer of Gallium Nitride (GaN) wafers in the US
- Soraa has invented a new reactor technology and process to produce GaN wafers at high quality and low cost
- Need to control dissolution / deposition of GaN & fluid flow pattern for optimum crystal growth



- Soraa has reactors capable of achieving "pilot" production quantities => currently optimizing crystal growth using empirical approach; requires long and expensive development crycle
- We seek to develop an accurate simulation model of crystal growth process to dramatically cut down on the lead time AND expense of scaling up to production
- LLNL has outstanding computational facilities and expertise in modelling of reactive flows; Soraa has a team of scientists & engineers with expertise in GaN crystal growth and apparatus design
- Low-cost GaN wafers will revolutionize solid-state lighting and power switching devices

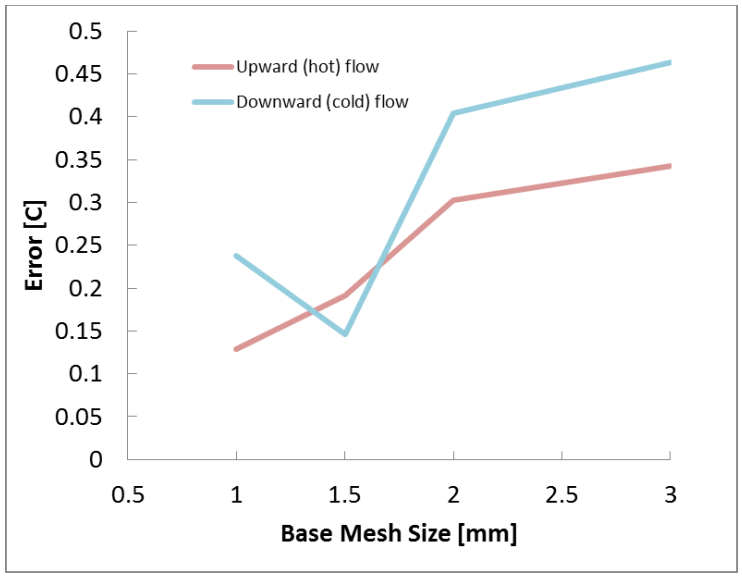
Technical Innovation

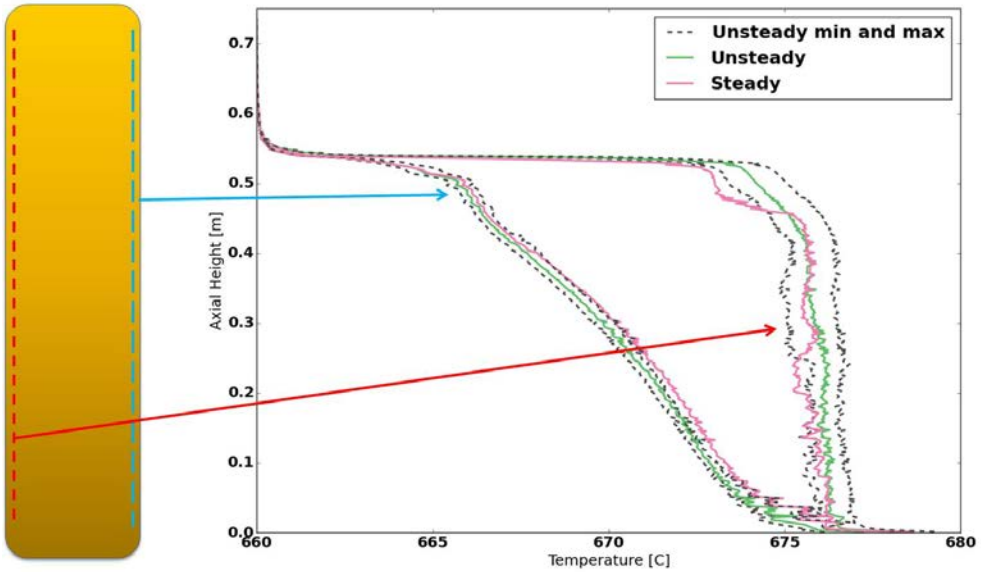
- Soraa has studied the effect of fluid flow on crystal growth using steady-state CFD simulations and a desktop computer (8 CPUs)
  - Fluid flows are inherently unsteady → transient calculations may be necessary
  - Including multiple effects such as chemical reactions, effect of dissolved species on fluid properties further compromises mesh resolution
- HPC allows us to include physics not possible on standard hardware
  - Ability to conduct a mesh convergence study to select grid resolution based on internal geometry
  - Transient calculations to capture the "true" average flow pattern
  - Testing of several turbulence models to identify best fit based on experimental comparison
  - Parameters to model chemical reactions are unknown → HPC allows many simulations to identify best-fit parameters (work in progress)

Technical Approach

- Soraa provides reactor geometry, process conditions , baseline simulation setup , experimental data and one of 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
- Approach for Phase I:
  - Assume dissolved species do not affect fluid properties
  - Extrapolate NIST data beyond 427 °C
  - Assume a single intermediate dissolved species
  - Iterate to identify “best-fit” rate constants for chemistry
- Soraa, as a leader in GaN-on-GaN LEDs, is uniquely positioned to take advantage of any cost or quality improvements in the supply of Bulk GaN wafers

Results and Accomplishments





- Documented best practices for CFD of natural convection problems
- Mesh convergence study identified 1.5mm grid size is adequate
- Transient analysis indicated that flow is quite unsteady and steady-state analysis may not give a good "average" representation of flow
- Currently working on adding chemistry to the model