Abstract

The HPC4Manufacturing Program is Department of Energy (DOE) Energy Efficiency and Renewable Energy (EERE) sponsored program with the aims of introducing industry to high performance computing for advanced science and engineering simulations, transferring advanced simulation techniques developed at the National Laboratories to industry and reducing industrial energy usage. The partner national laboratories have been working with a variety of large and small companies in a variety of energy intensive industries to improve manufacturing processes and enhance product design. Examples include optimizing steel-making furnaces to reduce energy and coke usage and advanced CFD modeling of turbines used for aerospace and energy generation. Many companies are interested in advanced simulation to reduce costs associated with product/or and process testing.

Keywords: High Performance Computing, Public-Private Partnerships

Introduction

The supercomputers at the National Laboratories are amongst the largest in the world. The laboratories have developed the scientific and computational expertise to effectively utilize this resource to address many of the most difficult scientific problems. In particular, high performance computing (HPC) is especially useful when addressing large problems at multi-scales such as understanding macro-properties of materials starting with atomic-level interactions or understanding processes that exist in high - temperature, harsh environments where instrumenting experiments is difficult. As computational resources increase in size and modeling software continues to capture the physics of processes more accurately, high performance computing enabled modeling and simulation will likely become a competitive advantage for those companies wishing to optimize product design and manufacturing processes.

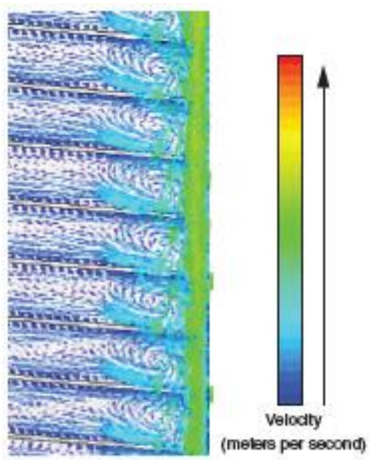
In recognition of the role that HPC could play in improving processes in industry and ultimately reducing energy usage, the Department of Energy (DOE), Energy Efficiency and Renewable Energy (EERE), Office of Advanced Manufacturing (AMO) is sponsoring a program called HPC4Manufacturing to encourage U.S. manufacturers to partner with the National Laboratories to use the computational expertise and infrastructure available at the laboratories to solve difficult manufacturing problems which could lead to increasing the energy intensity of products and processes. The intent of the program is to help foster collaborations between industry and the national laboratories and to help industry recognize the usefulness of HPC capabilities and to implement them more broadly in their business model. A sister program, HPC4Materials, has also been launched by DOE's Fossil Energy Office (FE), EERE Vehicle Technology Office (VTO), and Fuel Cell Technology Office (FCTO) to develop new materials.

Method for Industry Engagement

Industrial partners become involved in the program though a solicitation process. Solicitations are announced through the media and the program website (www.HPC4Mfg.org). Potential industrial partners prepare a two-page concept paper which is reviewed by a review committee. Selected proposers are then paired with laboratory personnel and together they write a full proposal that is reviewed by the review committee. The DOE sponsoring office makes the final funding decisions and provides up to $300K to national laboratory personnel to work with the industrial partner. Industrial partner is required to provide at least 20% of the project costs in in-kind or cash cost share. An example of a project funded by this program is described below.

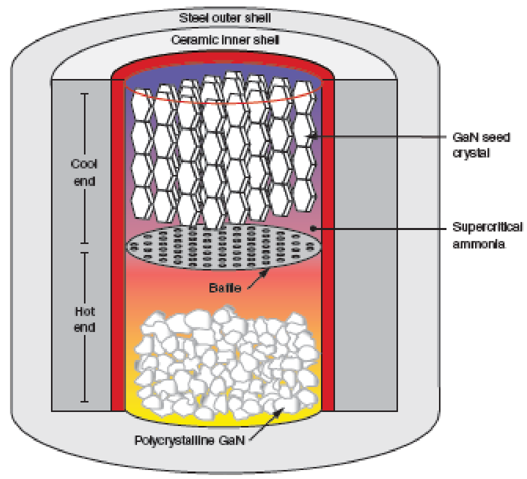
Example Project – SORAA

Researchers at Lawrence Livermore National Laboratory worked 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 was to help improve the crystal-growth process, leading to widespread adoption of GaN for substrates in solid state lighting and power electronics, among other 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.



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

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 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 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.



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

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.

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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