Optimizing the growth of semi conductor GaN crystals

GaN's atomic structure, a crystal, and an HVPE reactor where it is grown.

Supervisors:

- Prof. Olga Mula (TU Eindhoven, research website),
- Dr. Markus Zenk (Fraunhofer Institute IISB, Germany)

Location: Fraunhofer Institute IISB, Scientific Area: Semiconductor Technology, Department Materials, Schottkystrasse 10, 91058 Erlangen, Germany. [website]
Duration: 4-6 months.
Possibility to continue with a PhD after the master thesis: yes

Project's topic

Gallium Nitride (GaN) crystals are impressive. They are a basic material for fabricating optoelectronic devices such as LEDs (2014 Nobel Price in Physics for an efficient blue light emitting LED). They are also an attractive semi conductor for many different power electronic devices (e.g. fast chargers for consumer electronics and automotive). Due to these realized and prospected applications, GaN will play a significant role in future electronic markets. Yet growing bulk GaN crystals is very challenging. The main growth technique for the fabrication of bulk GaN crystals is currently the Hydride Vapor Phase Epitaxy (HVPE). Here, the crystals grow from precursor species that are transported to the crystal surface in their gas phase. The technology can be improved by optimizing the geometry of the reactors, and by finding the best operating conditions. Optimizing this whole process is very difficult because one cannot rely only on experiments: It would require too much time and is economically inefficient. Thus one resorts to numerical simulation but here again challenges arise:

- One needs to work with a good physical model. In this case, these are based on multi-species, compressible Navier-Stokes equations. Solving these models numerically is already challenging in itself regarding the discretization methods, and computations take a very long time (in the order of days).
- The model depends on many different parameters (e.g., diffusion coefficients, parameters for chemical reactions).

To optimize crystal growth, we are thus led to use the physical model to find the optimal parameter values, and reactor geometry yielding the best crystal growth. For this, optimization methods typically require solving the physical model for many different configurations, and one is thus confronted with long computational times.

The goal of this project is to make the whole optimization process viable by learning a surrogate model that maps the parameters to the PDE solutions and which can be evaluated quickly. This will require combining reduced modeling and machine learning techniques.

What will you learn?

A project of this type will allow you to learn a number of topics and skills:

- Modeling flows with Navier-Stokes equations,
- How to do shape and parameter optimization,
- How to mathematically describe the concept of compression,
- What are compression algorithms based on reduced modeling and machine learning to build the surrogate model, what are the current challenges in this field,
- You will also learn about the physics of GaN crystal growth, and how to interact with colleagues with different backgrounds (physics, chemistry)

What are the concepts that you already need to know before starting such a project?

The project is at the interface between computational PDEs, and engineering so you must have a taste for interdisciplinary work, and some knowledge in numerical methods for PDEs, and modeling. We will work with mathematical concepts for which there are advantages in describing them in an infinite dimensional setting. In other words, familiarity with the setting of Functional Analysis would definitely be a plus but it is not strictly necessary. Finally, some familiarity with optimization methods such as the basic gradient descent will be desirable. To summarize, the requirements are:

- Scientific Computing (2MMN10)
- Scientific Programming (2MMN20)
- Basic knowledge in optimization
- Good coding skills in Python and interest in coding
- Having taken the master courses on Applied Functional Analysis and PDEs is a plus.

Location and supervisors

The project will be supervised by Prof. Olga Mula (TU Eindhoven) and Dr. Markus Zenk (Fraunhoffer Institute, IISB). The master student is expected to work at the Fraunhofer Institute IISB in Erlangen, Germany, for a period of 3 to 6 months. The institute is on the campus of the Friedrich-Alexander University Erlangen.