

INTERNSHIP OFFER*Master 2 or 3rd year of engineering school***Development of modelling strategies for the Al/N-doped polycrystalline SiC Chemical Vapor Deposition process**

Duration	6 months, starting from February 2027
Location	Laboratoire SIMaP, 1130 Rue de la Piscine - BP 75 – 38402 Saint Martin d'Hères – France
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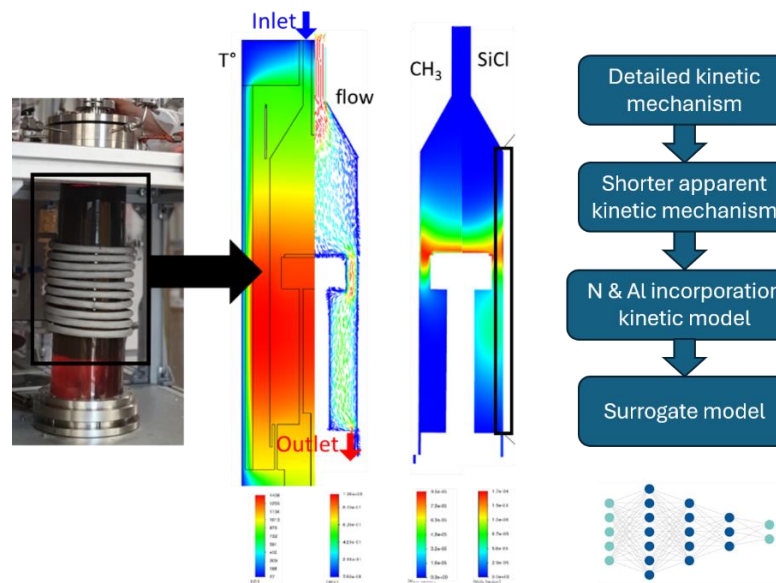
Context

Today, driven by ecological and geopolitical considerations, a large-scale electrification of society is envisaged as a way of reducing our dependence on fossil fuels, with power electronics components playing a key role in this transition. **Silicon carbide's** (SiC) exceptional physical properties make it an ideal candidate for the manufacture of these components which however depend on the availability of large single-crystal substrates of excellent crystalline quality, still considered too costly. A high-potential alternative strategy consists in transferring a thin film of **monocrystalline SiC** by **Chemical Vapor Deposition (CVD)** with controlled thickness, homogeneity and conductivity (thermal and electrical) onto a **polycrystalline SiC** substrate already produced by **Mersen**. Chemical Vapor Deposition is a complex process involving the transport of the reactive species (originating from the decomposition of precursors) inside the reaction chamber to a surface where the thin film of material grows under specific operative conditions. This process then couples transport phenomena, gas-phase reactions and surface reactions. Over the years, a strategy coupling modelling and experiments has been developed to better understand and optimize such processes. **High-fidelity simulation** of the **thin film growth rate** and **local partial pressures of reactive species** everywhere in the reactor is of particular interest since both factors govern the deposit's microstructure and resulting properties.

A set of CVD experiments has already been conducted under various operating conditions, providing the experimental database of this internship. This internship will focus on the process simulation part by using a commercial **Computational Fluid Dynamic (CFD)** code and then exploring the different strategies enabled by the recent advances in **artificial intelligence (AI)** and **machine learning (ML)**.

Objectives

In previous work, CFD simulations using a refined comprehensive SiC **deposition kinetic model** has been compiled in order to reproduce experimental data obtained in a lab scale reactor. However, for larger industrial CVD reactor, this approach becomes computationally too expensive and can no longer be effectively used to support the scale-up. Your primary objective will be to reduce this detailed mechanism into a shorter set of apparent reactions using an **automated optimization** approach, to simulate the first set of experimental data and find an optimum between computational efficiency and physical accuracy. Then, this strategy will be extended toward a second set of experimental data to simulate the **N/Al-doping of SiC** CVD thin films. Finally, **surrogate models**-based strategy of the process will be initiated to reproduce the two sets of experimental data.



Your mission will include:

- **Learning commercial CFD code provided by Ansys Fluent:** Setting up a CVD reactor model and interfacing with Python
- **Reviewing the literature:** compile kinetic scheme and rate constants from the literature + identify ML methodologies that could be used to make surrogate models.
- **Reducing the kinetic model via optimization approach:** Analyzing our current kinetic model and implementing numerical reduction techniques to derive apparent reaction steps, cutting down the number of active species and elementary reactions. Developing and executing custom optimization algorithms in Python to systematically evaluate, automate, and calibrate the reduced kinetic mechanism against experimental data.
- **Integrating doping in the mechanism:** Extending the kinetics optimization framework to Aluminum (Al) and Nitrogen (N) incorporation, both used as doping agent.
- **Developing surrogate Reactor Modeling:** Applying Machine Learning (ML) techniques to build a high-fidelity surrogate model of our CVD reactor, bridging traditional physics-based CFD with modern data-driven approaches to accelerate simulation time.

The internship will take place in the framework of a joint laboratory (CarbLab) between MERSEN company (<https://www.mersen.com/fr>) and SIMaP (<https://simap.grenoble-inp.fr/>), a research lab specialized in materials sciences and associated processes. Therefore, you'll have one foot in academia and the other one in industry, allowing you to see how these two can collaborate for tomorrow's new materials and process developments.

Profile & requested skills

We are looking for a highly motivated student (M2 or 3rd year of engineering school) with a background in materials sciences and/or process engineering with a strong interest in modelling work, programming, and AI/ML. The student must be dynamic, curious and autonomous. The student must speak French and/or English.