Optimization of Hydride Vapor Phase Epitaxy (HVPE) Deposition Reactor manufacturing III-V Materials using multiple Large-Eddy Simulations (LES)

Compared to traditional silicon-based solar cells, III-V materials possess several advantageous properties for photovoltaic applications. First, their large light-absorption coefficient allows for thin and lightweight solar cells, thereby enabling portable applications. Second, their conversion efficiency from light to electricity is superior to that of silicon-based materials. Metalorganic vapor-phase epitaxy (MOVPE) [1] is the preferred manufacturing process of III-V materials, as it has been successful at producing highly efficient solar cells [2]. However, this technique induces large manufacturing costs which make III-V materials viable only for specific applications. The large cost is due to the cost of the reactants used, and the rate at which the solar cells grow, which prevents industrial scaling of the technology.

An alternative process is the hydride vapor phase epitaxy (HVPE) [3] which has been shown to provide a growth rate two orders of magnitude higher than that of MOVPE, while using cheaper reactants [4]. The process has been recently refined into a dynamic-HVPE (D-HVPE) and has been shown to provide satisfying efficiency [5, 6]. Although promising, the faster growth rate of the solar cells and the cheaper materials used come with new manufacturing challenges that need to be addressed. The overarching objective of this work is to propose a design that will address these challenges and make D-HVPE viable in an industrial context. The specific challenges are described below:

- Thin film solar cells consist several layers, each one made of a different III-V compound. When the growth rate of the solar cell is low enough, the substrate can be kept idle in the same chamber while different reactants are injected over time. With a higher growth rate - such as in HVPE deposition reactors - this strategy can lead to a non-uniform composition in each layer, which is detrimental for the efficiency. To avoid this issue, here, the substrate is moved to a different chamber each time a new layer needs to be grown (see figure enclosed). Ideally, the chambers operate at the same time on a different substrate to maximize the throughput of the reactor. While efficient, this configuration poses a fluid dynamic problem: if the reactants of one chamber escape to a neighbor chamber, it could contaminate the layer grown in the neighbor chamber, thereby hindering the solar cell efficiency. Additionally, the deposition of reactants between chambers can create maintenance issues as the reactants are typically poisonous. The first challenge is to reduce the leak between chambers.

- In HVPEs, the gaseous halides used for the deposition are obtained by mixing HCl with the group-III metal (here, Ga or In) at high temperature. Since the products of the reaction need to be maintained at a high temperature, it is advantageous to have the chemical reaction occur inside the deposition chamber (see figure enclosed), while the chamber is externally heated. This step creates a complex fluid flow in the chamber due to the buoyancy effects. At the same time, reactants should be deposited fast enough to avoid spurious reactions, and should mix fast enough to ensure uniformity of the layer grown on the substrate. The second challenge is to find an injection scheme that will satisfy both conditions.

In this work, multiple large-eddy simulations are conducted to better understand the manufacturing challenges posed by D-HVPE deposition reactors, and improve their design. The simulations are run with a variable density low-Mach solver based on OpenFOAM [7]. The results are processed with different sensitivity analysis techniques including active subspaces [8] and Sobol indices [9] to identify the features that affect the most out-of-chamber leak and reactants uniformity on the substrate. The results of the sensitivity analysis are used to propose new designs and optimize the geometry of the deposition reactor. In the end, this work participates in the improvement of D-HVPE deposition reactors and will enable the emergence of portable photovoltaic applications in a variety of sectors.

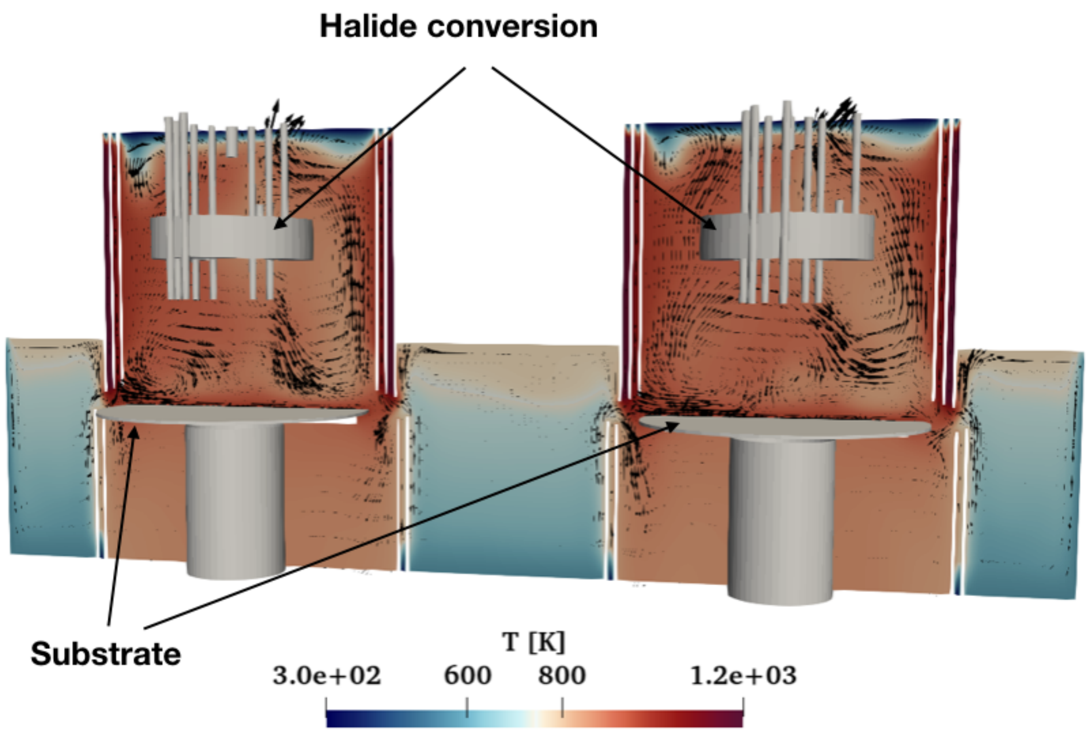

Figure 1: Contour of temperature in the HVPE deposition reactor. White elements denote the substrate, its support, and the reactant injection scheme. Arrows indicate the instantaneous orientation of velocity. Note that multiple substrates are operated at once in neighboring chambers, and that the gaseous halide is produced inside each chamber.

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