Future challenges for MOVPE – an industrial perspective

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This paper attempts to predict where the future challenges lie for MOVPE from an industrial perspective. These key challenges include the need to provide ever-increasing capacity and ever-reducing costs, the need to cope with increasing complexity and the tightening of tolerances, the need for device-level qualification, the shortening of product development cycles and the need to address environmental sustainability and recycling issues. The paper identifies two themes that the author believes are crucial to the resolution of these key challenges. The themes are those of “modeling and simulation” and “monitoring and control”.

1. Introduction
It was Niels Bohr, the Nobel laureate, who once remarked that “Predictions are always difficult, especially about the future”. Notwithstanding his comment, this paper will attempt to predict where the future challenges lie for MOVPE. It would be unrealistic to attempt to address all of the future challenges within a single coherent article, so the author has chosen to address this issue from a purely industrial perspective, and consequently from a shorter-term viewpoint. Hence, the principal views expressed in this article reflect the issues encountered within IQE (Europe) Ltd, a commercial foundry of custom compound semiconductor epitaxial wafers by MOVPE. Other views have been taken from co-workers in the MOVPE field and these contributions are duly acknowledged.

2. Some major challenges
The major challenges for an industrial MOVPE epitaxial-wafer operation can be summarized as follows:

1. Increasing capacity – This involves investing in larger and faster, or simply more numerous, MOVPE reactors (and associated equipment), larger production facilities and increased levels of automation.

2. Reducing costs – This is achieved through cycle-time optimization, yield improvements, materials efficiency improvements and improved monitoring and control systems.

3. Increasing complexity – Epitaxial layer structures will continue to increase in complexity in order to achieve higher levels of performance and increased functionality.

4. Tightening tolerances – In addition to the increasing complexity noted above, there is the requirement to continually tighten tolerances. Both aspects put considerable pressure on yields and often require new control systems to be introduced and improved characterization/monitoring techniques to be developed.

5. Device-level qualification – Increasingly the end user is not satisfied with materials characterization alone (i.e. layer thickness, doping, etc.) since this is not able to provide sufficient data to guarantee successful device operation. There is a need to provide device-level processing and testing to confirm that the epitaxial structure meets a device-level specification, giving the end user the confidence to commit the material to the production line. Often, the first indications of material quality, from the customer’s own production line, occur up to 3 months later, so the potential liability for both parties can be considerable. Hence, more direct methods must be developed by the epiwafer supplier to qualify the material prior to shipment.

6. Shortening product development cycles – In common with all high-technology businesses, the product development cycle is continually shortening. In the epitaxial wafer business this is epitomized by the need to rapidly introduce new materials, new layer structures and new device types.

7. Environmental sustainability and recycling – Last, but by no means least, is the need to continue to address the issues of environmental sustainability and to look toward material recycling. While there is no doubting the importance of this subject, it will not be considered further here due to limitations of space.

So, how do we address these challenges into the future? This paper identifies two themes that the author believes are central to the resolution of these key challenges. The themes are those of “modeling and simulation” and “monitoring and control”.

3. Modeling and simulation

According to Berardinis [1], “The future of the semiconductor industry doesn’t hinge on finding new materials or more efficient transistors. According to the equipments designers, it hinges on modelling technology”. There are various strategies for the application of modeling within the semiconductor facility. The three dominant strategies are process technology, equipment technology and factory operations. Process technology includes molecular-level chemistry and physics for the determination of growth rates and semiconductor alloy compositions. Equipment technology includes the use of steady-state computational fluid dynamics (CFD) studies. Finally, factory operations cover discrete event simulations and optimization/control algorithms. Modeling of the process and the equipment is currently limited by the commercial availability of the necessary sophisticated software models. Hence, at this stage, simulations are largely limited to factory logistics.

Commercial CFD programs provide a method for modeling flow dynamics, heat transfer and chemical reactions in both gas phase and surface phase. CFD has been the subject of significant research over the past 10–20 years, but more recently it has become an industrial activity in the MOVPE field due to the availability of robust, flexible and multi-disciplinary commercial packages focused toward this application [2, 3], combined with the lower cost of high-end computers necessary to run such software. At this stage, the software has been primarily employed to support equipment design (e.g. Aixtron, Emcore, etc.) but is becoming more common with MOVPE equipment users in order to understand and optimize their processes [4–7].

CFD programs provide first-principles prediction of gas flow, heat transfer and mass transfer. They provide a solution for the Navier–Stokes transport equations within 2D and 3D domains with a variety of boundary conditions. An MOCVD process model includes multi-disciplinary physics and chemistry such as thermal radiation transfer, induction heating and gas-phase and surface-phase chemistry. One of its most important uses is the accurate prediction of heat transfer, since the temperature of the internal surfaces controls chemical species in terms of diffusive properties, gas-phase reaction rates, surface-phase reaction rates and surface incorporation [5, 6]. Also important are details of the gas-delivery system such as the inlet nozzle design, which provides separate group III and V injection, avoids pre-reactions, removes vortices, and avoids deposition at the inlet area. As the group III and V injected gases travel from the nozzle over the heated wafer the various species decompose to produce the epitaxial layers. The depletion profile across the wafer is generally non-linear and often wafer rotation is employed to create a uniform epitaxial layer. Fig. 1 shows the depletion profile for an AlGaNAs layer grown in a 5 × 4” Aixtron multiwafer planetary reactor both with and without wafer rotation. The rotating wafer averages out the variations in growth rate along its diameter resulting in a more uniform layer thickness. By adjusting the total gas flow (Q_{tot}) it is possible to modify the shape of the depletion profile and thereby influence the layer uniformity. The agreement between modeled and experimental results is very good.

An exciting concept being developed by CFD Research Corporation is the Virtual Reactor Process Equipment Simulator [8]. The “VReactor” is a custom-built virtual copy of the real process chamber and it performs real-time analysis and post-processing of actual physical/chemical processes taking place during different chip manufacturing steps. “VReactor” is a customized CFD application comprising a developed set of chemical kinetics reactions and thermodynamic data from SRI International. “VReactor” embodies a model-based simulator that is able to emulate equipment behavior with process controls, much like the well-known flight simulators, using advanced physical models. The simulator ideally offers an interface that mimics the hardware itself and provides a direct real-time visualization of the processes occurring within the equipment. The benefits of such a simulator are numerous; it helps to sell/demonstrate products to clients, it provides an excellent way to train operators, it enables operators to experience equipment behavior...