Computational Fluid Dynamics modeling of a Novel High-Pressure Spatial Chemical Vapor Deposition Reactor (HPS-CVD) Design for Growth of Indium-Containing Nitrides

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Epitaxial growth of high-indium-content nitrides, such as $In_{1-x}Ga_xN$ or $Al_xIn_{1-x}N$, is challenging due to the relatively low dissociation temperature of InN into indium metal and nitrogen gas necessitating growth temperatures which are sub-optimal for growth of device-quality films.[1] Increasing the gas pressure (up to 15 atm) within a horizontal flow metal-organic chemical vapor deposition (MOCVD) tool has been shown to be effective at increasing the growth temperature of InN and at increasing the indium incorporation at a certain growth temperature.[2] Unfortunately, higher pressures and resultingly higher fluid densities result in fluid dynamic and heat transfer challenges which result in turbulence and loss of group-III source material prior to incorporation on the substrate.

To address the fluid dynamic challenges associated with high-pressure MOCVD growth of (nitride) materials, a new MOCVD reactor has been proposed which carries the potential to operate at super-atmospheric pressures (up to 100 atm).[3] Key to this innovative design is the spatial separation of precursors prior to mixing in the boundary layer immediately above the substrate.

This contribution will discuss the current state of development of this tool via a discussion of computational fluid dynamic simulations performed using the computational fluid dynamics software, COMSOL Multiphysics. Fully coupled flow and thermal studies of this novel high-pressure spatial chemical vapor deposition (HPS-CVD) tool will be presented and suitable operating windows for super-atmospheric conditions discussed to highlight the viability of this platform.

References:

[1] Yamamoto, A., Sugita, K. & Hashimoto, A. Elucidation of factors obstructing quality improvement of MOVPE-grown InN. *J Cryst Growth* **311**, 4636–4640 (2009).

[2] Dietz, N. *et al.* The growth of InN and related alloys by high-pressure CVD. *Proceedings of SPIE* **5912**, 59120E-59120E–8 (2005).

[3] Yousefian, P. & Pimputkar, S. Computational fluid dynamics modeling of a new high-pressure chemical vapor deposition reactor design. *J Cryst Growth* **566**, 126155 (2021).