Influence of Natural Convection and Thermal Radiation on Multi-Component Transport and Chemistry in MOCVD Reactors

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Introduction

The combined effects of radiation and natural convection on the growth of electronic materials in Metal Organic Chemical Vapor Deposition (MOCVD) reactors are currently being investigated by CFD Research Corporation and NASA Langley Research Center (LaRC) under NASA microgravity research project NAS8-40846.

In the first phase of the study, infrared data were obtained at LaRC for a sled reactor using pure gases. The system was then modeled using the CFD code, CFD-ACE, and the prediction validated against empirical data [Kannapel, 1997]. Following these pure gas simulations, the current focus of the study is to model a fully reacting MOCVD system. For this phase, data for the growth of Indium Phosphide at the University of Virginia (UVA) are being used for comparison [Black, 1993].

Experimental Set-up

The experimental apparatus used for the thermal studies is located in the Chemical Vapor Deposition Facility for Reactor Characterization at NASA Langley Research Center [Johnson, 1991]. The reactor has a circular inlet section that feeds the reactants into a rectangular duct in which is mounted a fused silica sled containing a graphite susceptor. The graphite susceptor is heated by an external Radio Frequency (RF) induction coil, wound around the outside of the silica test section. A similar reactor is in use at the University of Virginia. This is the commercial Crystal Specialties Model 425 MOCVD reactor used to obtain the InP data used for the current model validation [Black, 1993].

MOCVD Computational Model

The above MOCVD systems are modeled using the computational fluid dynamics code CFD-ACE. The solution domain consists of the entire reactor including the chamber, the graphite susceptor, the fused silica walls, and the fused silica susceptor holder. The model solves for the heat and mass transport within the reactor and also computes the coupled gas phase and surface chemistry.

Preliminary Test Case

The initial UVA test cases selected for validation of the CFD-ACE model are for the deposition of Indium Phosphide (InP) from the precursors Phosphine (PH_3), Trimethylindium ($In(CH_3)_3$), and Monomethylindium ($InCH_3$) with Hydrogen as the carrier gas. The following reaction set is assumed for this system [Black, 1993]:

Surface

$$In(CH_3)_3 + PH_3 \rightarrow InP(s) + 3CH_4$$

$$In\,CH_3 + PH_3 \rightarrow InP(s) + CH_4 + H_2$$

Gas Phase

$$In(CH_3)_3 \rightarrow InCH_3 + 2CH_3$$

The current set of numerical predictions for the UVA InP system are shown to compare well with simulations performed by Black. Both set of results match well with the experimental data at lower pressures (e.g., 0.1 atmosphere) but diverge from the experimental data at 1 atmosphere. This pressure dependence discrepancy has also been seen in modeling predictions for the growth of GaAs [Jansen, 1991; Black, 1991]. The possible reasons for this pressure dependent discrepancy are discussed. They include parasitic deposition, morphological effects, and gas phase/surface reaction mechanisms. Plans for further isolation of the cause are presented.

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