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A Modular Simulator Development Approach for the Design of GaN CVD Systems

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Abstract

A novel approach to GaN CVD equipment simulation, developed as part of a joint research program between the University of Maryland and Northrop Grumman Corporation, will be discussed in this paper. An alternative to the "traditional" (e.g. CFD-based) approaches to high-fidelity equipment simulation was developed, motivated by the need for flexible simulation tools that would allow the rapid evaluation of reactor design alternatives and that interface readily with available optimization, process control, and numerical analysis tools. The overall goal of this research program was to optimize GaN CVD reactor components to improve thickness and composition uniformity across the wafer.

Gallium nitride (GaN) is a compound semiconductor material with physical and electrical properties that include a low dielectric constant, high breakdown voltage, high melting point, and high thermal conductivity. These properties make GaN an attractive material for manufacturing high-power and high frequency (1-50 GHz) power transistors for communications and radar applications.

Despite the potential of these applications, GaN devices remain out of reach of most commercial applications because of the numerous difficulties associated with manufacturing GaN films. For example, in metalorganic vapor phase epitaxy (MOVPE) processes, precursor chemical species for the III and V compounds can react spontaneously to form adducts that may lead to further undesirable reactions, depositing Ga-containing compounds in the gas delivery system and elsewhere in the reactor, depleting the reactant gas of the intended deposition species. Attempts to reduce or otherwise control these gas phase reactions have given rise to numerous CVD reactor designs. For example, vertical, single-wafer reactor designs with separate single [SRK] and multiple [PTSMMST], [TMMH] injectors for the different precursors have been developed by University of Wisconsin and SUNY/Sandia/Thomas Swann researchers, respectively, in an attempt to reduce gas-phase reactions and control film-thickness uniformity. Horizontal single wafer [KN] and commercial multiple-wafer [BSWSMHDJ] systems also have been developed, and in the latter case, extensively optimized to produce spatially-uniform films. Non-thermal deposition modes including photo-electric assisted [TRNK], heated-filament assisted [BRHCHJ], and plasma-enhanced [BLC], [LCB] CVD modes also have been pursued for GaN CVD.

In many of these studies, extensive simulation work was performed to understand gas phase reactions and to tune operational or design parameters of the reactors with the goal of minimizing thickness nonuniformities in the deposited films. Those studies focusing on quantitative simulation of gas phase reaction chemistry (e.g., [SRK], [PTSMMST], [TMMH]) conclude that some of the details of the gas-phase reactions actually do not play an important role in determining film thickness variations; deposition rate appeared to be determined primarily by the flux of all Ga-containing species at the wafer surface.

In this paper, a novel approach to GaN CVD equipment simulation, developed as part of a joint research program between the University of Maryland and Northrop Grumman Corporation, will be discussed. An alternative to the "traditional" (e.g. CFD-based) approaches to high-fidelity equipment simulation was developed, motivated by the need for flexible simulation tools that would allow the rapid evaluation of reactor design alternatives and that interface readily with available optimization, process control, and numerical analysis tools. The overall goal of this research program was to optimize GaN CVD reactor components to improve thickness and composition uniformity across the wafer.

As a result of these requirements, modular simulation elements were developed to describe the reactant gas velocity and pressure profiles within the showerhead and in the reactor chamber. Initial efforts were focused solely on transport of Ga-containing species to the wafer surface, with showerhead design optimization based on improving the uniformity of flux of these species at the wafer surface. Chamber heat transfer modules were developed to describe gas and reactor chamber component temperatures. Object-oriented programming concepts were used to define object classes corresponding to the CVD reactor physical components, as well as sets of operating conditions for the process. Other simulator components were developed from the abstraction of boundary-value problem based model solution (global spectral) methods and other underlying numerical methods for solving the nonlinear equations originating from the energy and chemical species transport equations.

The resulting simulator library was found to be effective at indicating the reactor design features to which thickness uniformity was most sensitive. The physically based simulation approach was useful for gaining insight into the physical and chemical mechanisms responsible for across-wafer non-uniformity and wafer-to-wafer inconsistencies. The flexibility built in to the simulation methodology from the outset proved critical to enabling a relatively rapid simulation/experimental evaluation/redesign cycle, which was typically on the order of months. Significant deposition uniformity improvements were achieved after approximately three such iterative redesign cycles.

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