609a Gallium Nitride Thin Film Growth Chemistry Modeling and Experimental Validation within a Movpe Reactor Showerhead System

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Gallium Nitride (GaN) is a compound semiconductor material that has shown tremendous potential in electronic and optoelectronic devices over the past few years due to its wide-bandgap and high breakdown field properties. Metalorganic vapor phase epitaxy (MOVPE) is the principal method used to grow single-crystalline layers of this material. Currently, a wide range of reactor designs are used to manufacture gallium nitride devices. This indicates a lack of a coherent framework on how to design gallium nitride reactors for optimal single wafer and multiple-wafer production. Collaboration between the University of Maryland and the Northrop Grumman Corporation was initiated to help optimize GaN CVD reactor components, improve thickness and composition uniformity across the wafer, and enhance the limited understanding of gallium nitride deposition chemistry.

The accurate prediction of epitaxial thin film properties requires a complete knowledge of the chemical kinetics that occurs in the gas phase and at the surface. The choice of reactor operating conditions and physical designs has a significant influence on the selectivity among different reaction pathways, as is the case in GaN where two competing reaction pathways exist. The intricate adduct formation pathway produces high molecular weight adduct species which are believed to ultimately breakdown into large amounts of GaN and methane molecules. On the other hand, the thermal decomposition pathway of TMG is relatively well known with products being low molecular weight sub-alkyls. The extent to which these pathways occur is a function of reactor geometry, operating conditions, and the degree of precursor mixing as determined by the design of gas delivery systems.

A detailed chemistry model was developed and applied to a GaN MOVPE reactor showerhead system. A physically based model describing heat transfer and gas transport through the showerhead was previously developed and used in conjunction to this chemistry model to predict the distribution of gallium-containing chemical species in various reactor elements. All simulations were performed using object-oriented programming concepts using quadrature grid weighted residual method techniques. This paper will demonstrate both qualitative and quantitative validation of the chemistry model to deposition experiments. Moreover, this study provides further insight into the physical and chemical mechanisms underlying gallium nitride epitaxial film growth.