Analysis of carbon nitride growth in pedestal reactors by chemical vapor deposition

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Abstract

The chemical vapor deposition of polycrystalline carbon nitride in stagnation flow reactors is simulated. A model is used to predict the gas phase chemistry, temperature and velocity profiles, potential gaseous film growth precursors, and to evaluate the likelihood of bond rearrangement occurring in the bulk phase or on the deposition surface once the gaseous precursors are adsorbed. Numerical studies are carried out to predict the effects of inlet and substrate temperatures, reactor pressure, and inlet gas composition on the gas phase chemistry. Potential gaseous film growth precursors of carbon nitride are determined by quantitatively comparing the calculated results against existing experimental data. Results of the model indicate that the gas phase chemistry, including the gas composition at the deposition surface, is strongly affected by reactor pressure and inlet gas composition. However, the gas composition at the deposition surface does not depend strongly on the inlet temperature, while it is found to be strongly dependent on the substrate temperature. Since no correlation is found between the predicted near-surface concentrations of potential film growth precursors and experimentally measured bond types in the carbon nitride films, the experimentally measured bond types in the films must therefore result from chemical bond rearrangement occurring on the deposition surface or in the bulk phase once the gaseous precursors are adsorbed. Comparison between the calculated film growth rate using potential growth precursors and experimental data indicates that the CH_x (x = 0,2,3), C_2H_2, NH_x (x = 0,1,2), and H_xCN (x = 1,2) species are the most probable crystalline carbon nitride growth species. Among these, C and CH_3 dominate the carbon contribution to the film growth, and N is the primary nitrogen bearing species responsible for the film growth. The sum of predicted film growth rates for carbon bearing species is comparable to the experimentally determined film growth rate.

Keywords: carbon nitride, chemical vapor deposition, simulation