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Plasma Simulation of Si_3N_4 CVD Process

Si_3N_4膜のCVDシミュレーション

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The plasma produced by a microwave source is discussed based on a simulation using a multiphysics coupled 2 dimensional fluid model. The technological aspects in a silicon nitride chemical vapor deposition (CVD) process using a disilane and ammonia mixture are addressed. The model includes the incompressible Navier–Stokes, the multiple convection and diffusion transport modules, the convection and conduction heat transport for gas and electron temperature, and the transverse electromagnetic wave propagation for a planar microwave source structure coupled to the plasma. The chemical reactions used in this simulation were prepared based on quantum chemical calculation. The dominant precursors, deposition rate and mechanisms, and performance of the CVD process in terms of the film properties are investigated. Distributions of the ionic and radical species are calculated and the simulation results are correlated with experimental data. The significant impact of the surface reactions with the involvement of H, NH, and NxHy radicals and ions were established.

1. Introduction

Microwave plasma sources (MWPS) are widely used in thin film technology and understanding the phenomena involved in materials processing by MWPS is important in order to provide full control of the source performance and its design. Recently, the plasma processing, configurations, and characteristics of various plasma reactors were studied[1–2] and in particular an MWPS has been shown to achieve good process performance. For this type of system the gas mixture composition is one of the critical factors in controlling the deposition rate and film properties. In this work, the investigation of a disilane (Si_2H_6) with ammonia (NH_3) plasma produced by MWPS is done by simulation means. The 2D plasma fluid within multiphysics coupling (FEM framework) model was formulated for a 300mm wafer reactor. Extensive studies were done in previous works on numerical modeling and silane chemistry by several authors.[3–5] Although, disilane and higher silanes are produced in a silane plasma, to our knowledge similar work has not been reported for disilane as a working gas or in mixture with other gases.

In this paper, we will describe a model consisting of the coupled modules for calculations of the wave propagations, reactive gas and plasma transports, and energy balances.[6]

2. Model

The investigated CVD system consisted of a cylindrical reactor (ϕ 45 cm□x 20 cm, see Figure 1) equipped with a planar MWPS, annular gas feeders, and a ϕ 300 mm heated wafer stage. The MWPS is composed of a coaxial waveguide (CWG) and a planar slot antenna separated by a dielectric window from the plasma zone.

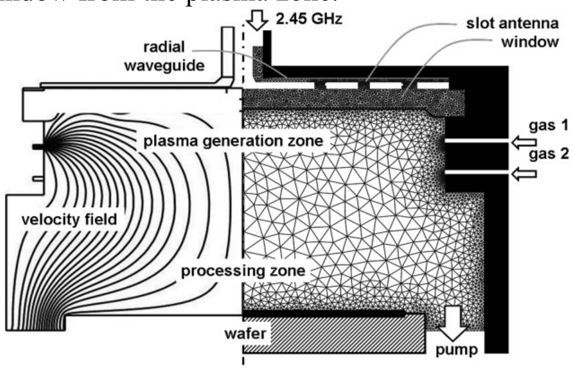

Fig.1. Configuration of microwave plasma reactor

The TEM mode which is excited by a 2.45 GHz generator propagates from the CWG through the planar radial waveguide and penetrates into the reactor through slots in antenna. The details on slot arrangements and their structure is not discussed in this work. We formulated a plasma fluid model with mutual coupling between individual variables associated with the reactor physics and chemistry. The reaction chemistry and film growth model are shown in Figure 2.

We examined the mixture of $Si_2H_6/NH_3(N_2)/Ar$ by the developed model. In the simulation the individual gas components were fed from the upper

(NH_3) and lower (Ar with Si_2H_6) gas feeders located in an annular fashion on the side wall (Figure 1) and the gas was evacuated through the pumping port located at the lower side of the plasma reactor.

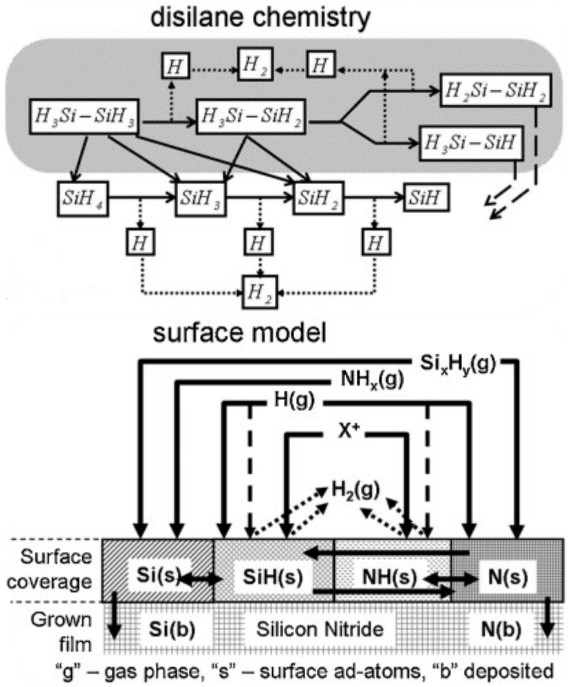

Fig.2. Reaction chemistry and film growth model

3. Results and Discussion

The actual modeling results generated a robust dataset, which had explicit and valuable impact on the tool development. The computed raw data were used to create the simulative diagnostics sheets (SDS) in order to perform cumulative and statistical analysis for each particular conditions. The SDS consisted of the comprehensive characterization and specification about the particular process, including fluxes, deposition rate, film composition, etc. and they were found very useful and practical for process engineers to validate computed results. In respect to experimental processing results, we believe that the simulation results represented reasonable values of plasma parameters and composition.

We observed that a significant amount of the molecular hydrogen and nitrogen were produced in the Si_2H_6/NH_3/Ar plasma. N and H radicals were generated in the whole volume of the plasma reactor via various gas phase chemical reactions. Despite the differences in plasma sources between MWPS and RF CCP[4] for both cases it was observed that most of the hydrogen was located in the center. The disilane was shown to be an efficient source of the radicals as the chamber volume was filled with species such as Si_2H_4, Si_2H_2, SiH_3, NH_2 and NH. On the other hand, the species Si_2H_6, SiH_4, SiH, NH_3, N_2 or H_2 have increased concentration closer to the gas inlets and dissociate when propagating into the bulk plasma.

The idea on the competing processes of volatilization of H(s) versus successive insertion into Si–Si(g) bonds by hydrogen flux toward the surface still needs further investigation for disilane plasma. More comprehensive understanding of these surface processes can be gained by sophisticated surface models or from molecular dynamics simulations.

Nevertheless, many diverse modeling aspects were tested within the computation process. We can conclude that the approach based on multiphysics coupling under FEM framework gave us an opportunity to study complex chemistry in a model with mutually coupled variables within reasonable computation times, characterize the complexity of the involved chemistry, and investigate the role of the numerous species such as $N_xH_y^m$ and $Si_xH_y^m$ (m = 0 or +) in film growth.

4. Conclusion

From the industrial and engineering aspects, we see an advantage of using a modular and flexible model with integrated multiphysics coupling that allows one to generate results within reasonable time to sustain either hardware or process development. The technologically rich and valuable information was obtained by a simulation using the described model with mutually coupled variables that are associated with various aspects of the investigated configurations and chemistry.

5. Acknowledgements

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