

Reactor scale multiphysics simulation studies of inductively coupled SF₆ & O₂ plasmas

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Abstract: In this study, a numerical modeling analysis of the gas-phase decomposition of pure SF₆ and SF₆/O₂ mixtures, in the presence of silicon was performed. The etcher has an axi-symmetric shape and two-dimensional model was considered to represent the process. It has a multi-turn rf coil around the dielectric plasma chamber and 13.56 MHz rf-power is inductively coupled to the plasma by transformer action.

Simulation studies have been carried out for SF₆ & O₂ at process 15 mTorr, 2000 Watt, -100 V dc bias and 65 sccm gas flow. Equal proportion of SF₆ and O₂ is taken. Process parameters are defined and the associated multiphysics modules such as flow, heat transfer, plasma, chemistry, electric and magnetic are judiciously tuned using multiphysics module. It is observed that the electron temperature decreases with increase in process pressure and also there is a decrease in no. density of electrons

1. INTRODUCTION

Reactor scale models that predict process responses as a function of plasma process parameters are an important part of deep reactive ion etching process development. Etching is a widely used method for the fabrication of semiconductor and micro-electro-mechanical systems (MEMS) for the realization of high aspect ratio microstructures having narrow features and to reach greater anisotropy of etched profiles [1]-[4]. Depending on the gas mixture used for the plasma production, different processes like film deposition, etching, polymerization, and activation can be performed in order to modify the first surface layers of a material.

Plasma etching process for micro-fabrication is regarded as a very intricate application because of the complicated physical and chemical process. Due to this reason, the optimized process parameters for etching are usually found through trial and error test runs which are quite time consuming. However, this problem can be overcome if a systematic and efficient approach is employed for achieving the optimum process parameters. Keeping this problem in mind, a simulation model has been developed that takes into account the relationship between controlled characteristics of inductively coupled plasma source and operating process parameters for Silicon film etching using SF₆&O₂.

2. PLASMA SIMULATION STUDIES

2.1 Process Description

Plasma process simulation studies have been carried out for ICP etch process chamber as shown in Fig. (1) which is a simplified model of the multiplex plasma etcher from Surface Technology Systems Co. It has a multi-turn rf coil around the dielectric plasma

chamber and 13.56 MHz rf-power is inductively coupled to the plasma by transformer action and plasma acts as a single turn lossy conductor. The etcher has an axi-symmetric shape and two-dimensional model was considered to represent the process.

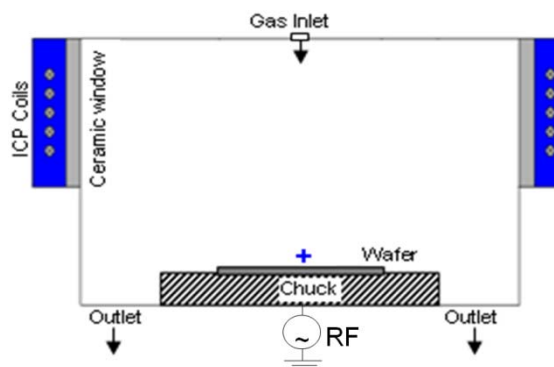


Fig 1: Schematic-ICP etch process chamber

2.2 Software Description

The multi-scale solution is made possible using the different ESI-CFD modules as shown in Fig. (2). Virtual prototype of the reactor is designed and discretized into finite volume elements using CFD-GEOM over which the flow equations are integrated. CFD-GEOM provides two classes of cells: structured and unstructured. The output file is written in dtf format. The resulting dtf is the used as input to CFD-ACE+. It is used for defining all the boundary conditions and volume conditions of the problem. It consists of various multiphysics sub modules like flow, heat transfer, plasma, chemistry, electric & magnetic field. All the required input parameter values required by these modules are defined and equations are solved using the solver. Solver gives output values of ion & radical no. density, ion & radical flux density, electron temperature, electron number density, power dissipation, electric &

magnetic field distribution, pressure distribution, electron and ion mobility inside the reactor. These values can be seen using post processing tool. CFD-VIEW.

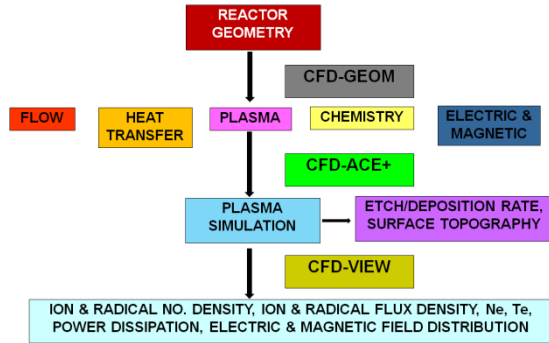


Fig 2: Schematic-Multiphysics modules used for Simulation

2.3 Mathematical Model

Developed plasma etch process simulator consists of equations from Flow, Heat Transfer, Chemistry, Plasma and Electric and Magnetic field module. Complete description of all the above equations is difficult and solving them as a whole is impractical. Hence simplified model is used for simulation purpose.

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho V) = 0 \quad (1)$$

$$\rho \left(\frac{\partial V}{\partial t} + V \cdot \nabla V \right) = -\nabla p + \mu \nabla^2 V + f \quad (2)$$

$$\frac{\partial \rho h}{\partial t} + \nabla \cdot (\rho V h) = \nabla \cdot (k \nabla T) + \frac{\partial p}{\partial t} \quad (3)$$

$$\text{Where } h = i + \frac{p}{\rho} + \frac{1}{2}(u^2 + v^2 + w^2)$$

$$\partial n_e / \partial t + J_e = S \quad (4)$$

$$J_e = \mu_e n_e \nabla \phi - D_e \nabla n_e \quad (5)$$

$$\frac{3}{2} \frac{\partial}{\partial t} (n_e T_e) + \nabla \cdot \left(\frac{5}{2} T_e J_e - \frac{5}{2} n_e D_e \nabla T_e \right) = J_e \nabla \phi + P_{\text{ext}} - L \quad (6)$$

$$n_e = \sum q_i n_i \quad (7)$$

$$J_i = -\rho D_i y_i + \rho y_i u_d \quad (8)$$

$$u_d = E (q_i \mu_i - \sum q_j \mu_j y_j) \quad (9)$$

$$E = -\phi - \partial A / \partial t \quad (10)$$

Equation (1) describes the conservation of mass, i.e. there is no loss or gain of mass in the system. Conservation of momentum is described by equation (2). The time rate of change of momentum equals the sum of the forces on the fluid. Here f represents

"other" body forces (forces per unit volume), such as gravity or centrifugal force and μ is the dynamic viscosity. Heat transfer processes are computed by solving the equation for the conservation of energy. This equation can take several forms and CFD-ACE+ numerically solves the energy equation in the form known as the total enthalpy equation. where h is the enthalpy, i is the internal energy as a function of ρ and T , k is thermal conductivity of the material, p is static pressure, u , v , and w are the moving speed of the molecules at x , y and z directions.

Equations (4)-(7) describes the transport equations for electrons, neutrals and radicals. Here n_e is the electron number density, J_e is the electron density flux, and S is the source of electrons produced or consumed in chemical reactions, μ_e is the electron mobility, D_e is the diffusion coefficient and ϕ is the electrostatic potential, T_e is the electron temperature. Parameters y , ρ , and D denote the mass fraction, mass density, and diffusion coefficient respectively in equation (8).

Equation (8) & (9) denotes the transport equation for ions where u_d is the drift velocity. The electric and magnetic field is computed according to equation (10) where ϕ & A denote the electrostatic and vector magnetic potentials respectively which are obtained by solving the Maxwell's equation in the frequency domain.

3. CHEMISTRY

The mass balances for the ions and radicals are solved in the chemistry module. Chemical reaction consists of gas phase (Table 1) and surface reactions (Table 2) for the plasma [5].

Table 1. Subset of Gas phase reactions for SF₆&O₂ plasmas and coefficient

| Reaction | A | n | E/R |
|---|-----------|---|------|
| SF ₆ +e→SF ₆ +e | 0 | 0 | 0 |
| S+F ₂ →SF+F | 2.9E-019 | 0 | 0 |
| 2SF→SF ₂ +S | 2.52E-017 | 0 | 0 |
| SF ₄ +F ₂ →SF ₅ +F | 2.63E-017 | 0 | 7346 |
| O ₂ +e→O ₂ ⁺ +2e | 9E-016 | 2 | 0 |
| O ₂ +e→O+O- | 8.8E-017 | 0 | 0 |
| SO ₂ +2F→SO ₂ F ₂ | 2E-033 | 0 | 0 |

The rate coefficients are assumed to have an Arrhenius form described by equation (11) where A = pre-exponential constant; n = temperature exponent; E/R = activation temperature; m = exponent on pressure dependency. Here k is expressed in kmol/m³s.

$$k = AT^n(P/P_{atm})^m e^{-E/RT} \quad (11)$$

The plasma reactions are governed by the collision of electrons with neutral and ionic species. Reactions between heavy particles are rare compared to electron-impact reactions. For an electron-impact reaction, the most fundamental information is the collision cross-section of the reaction. CFD-ACE+ also accepts the cross section data but converts to Arrhenius-type reaction rate data internally.

Table 2. Subset of surface reactions for SF₆&O₂ plasmas and sticking coefficient

| Reaction | A | E/R |
|--|---------|------|
| F+0.25SI(B)→ 0.25SIF ₄ | 0.116 | 1250 |
| F+0.5SI(S)→ 0.5SI_F2(S) | 0.2 | 0 |
| O→ 0.5O ₂ | 0.00035 | 0 |
| F ⁺ +0.5SI(S)→ 0.5SI_F2(S) | 1 | 0 |
| O ₂ ⁺ +SI(B)+2SI_F2(S)→ O ₂ +SIF ₄ +2SI(S) | 1 | 0 |
| F ⁺ → F | 1 | 0 |
| SF ₃ ⁺ +e→ SF ₃ | 1 | 0 |

4. RESULTS AND DISCUSSIONS

Simulation studies have been carried out for SF₆ & O₂ at process 15 mTorr , 2000 Watt , -100 V dc bias and 65 sccm gas flow. Equal proportion of SF₆ and O₂ is taken . Using the simulator, the behavior of electron temperature and electron density is studied as shown in Fig. 3.

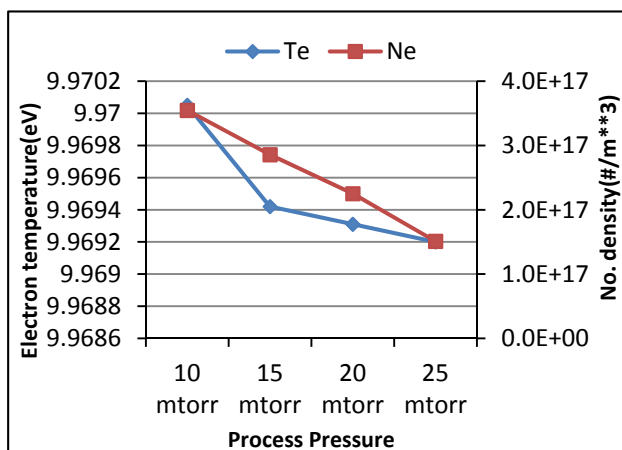


Fig 2: Electron no. density & electron temperature distribution w.r.t pressure at 65 sccm gas flow, 2 kW rf power and -100 V dc bias

It is observed that the electron temperature decreases with increase in process pressure which is due to the decrease in the mean free path and hence more number of collisions that lead to a decrease in

average electron temperature at constant power and also there is a decrease in no. density of electrons.

5. CONCLUSION

Developed simulation model provides reasonable results in terms of the number density & electron temperature distribution for SF₆&O₂ gas. It has been demonstrated numerically that electron number density and electron temperature is observed to be effected by the pressure.

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