Comprehensive Reactor, Plasma, and Profile Simulator for Plasma Etch Processes

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Abstract

In order to achieve predictive modeling results for plasma etching processes the effects of reactor, plasma, etch chemistry, and surface kinetics have to be taken into account concurrently. The new simulator was successfully tested on a case of polysilicon etching in a He/Cl_2 chemistry.

1. Introduction

In the recent years a lot of attention has been paid to modeling of plasma etch profiles [1-5]. Etch profiles, etch rates, and their uniformities across the wafer are the main concern of process engineers. Since they depend on reactor and plasma conditions, the modeling of etch profiles has to take into account proper equipment and plasma modeling. To address this issue the profile simulator SPEEDIE (Stanford Profile Emulator for Etching and Deposition in IC Engineering) was interfaced with HPEM (Hybrid Plasma Equipment Model) from the University of Illinois. Modeling results were experimentally verified, using trenches and overhang test structures for a He/Cl_2 chemistry in a conventional commercial RIE etcher.

2. Simulator

The modules of the simulator are shown in Fig. 1. Fluxes of etching radicals and ions are predicted by using a 2-dimensional (cylindrically symmetric) computer model HPEM [6,7], which combines modules which address either different physical phenomena or different time scales in an iterative fashion. The HPEM is composed of a series of modules which are iterated to a converged solution. The electromagnetic module (EM) generates inductively coupled electric and magnetic fields in the reactor. These fields are then used in the Electron Monte Carlo Simulation (EMCS) module. In the EMCS electron trajectories are followed for many RF cycles producing the electron energy distribution as a function of position and phase. These distributions are used to produce electron impact source functions, which are transferred to the Fluid Kinetics Simulation

module (FKS). In the FKS, continuity and ion momentum equations are solved for all neutral and charged particle densities, and Poisson's equation is solved for the electric potential. The FKS also imports an externally generated advective flow field produced in a hydrodynamic module (HM). The HM is a solution of the fully compressible fluid conservation equations for continuity, momentum, and energy. Slip boundary conditions may be used to extend the fluid equations to low pressure (5-20 mTorr). The plasma conductivity produced in the FKS is passed to the EM, and the species densities and time dependent electrostatic potential are passed to the EMCS. The modules are iterated until cycle averaged plasma densities converge. Acceleration algorithms are used to speed the rate of convergence of the model. For inductively coupled plasma (ICP) systems, all modules are employed. When simulating RIE systems, the EM is not used.

A circuit model is employed to self-consistently compute the DC bias of the powered electrode. Control surfaces are drawn at the boundaries of all driven or grounded metals. The conduction current (particle fluxes) and displacement currents passing through these surfaces (which may be inside dielectric materials) are computed on a cycle by cycle basis. The net currents flowing through these surfaces are then used to charge a blocking capacitor in series with the voltage generator. since the charging time for the blocking capacitor may be long compared to the simulation time, the size of the blocking capacitor is dynamically changed during the simulation.

The HPEM also includes a semianalytic model in the HPEM to address conditions where the mesh spacing, Δx, exceeds the actual sheath thickness, λ_s, at the boundaries. If the mesh is too coarse to resolve the sheath, the apparent sheath thickness is that of the mesh spacing adjacent to the wall. The sheath voltage is then dropped across the width of the numerical cell. In not resolving the sheath, the electric field in the sheath is diminished by the ratio of $\lambda_s/\Delta x$. To compensate for this effect in the HPEM, we separately compute the conduction and displacement current j_d to each location on the plasma-material boundary. With knowledge of the plasma density adjacent to the sheath we can compute the expected RF sheath amplitude thickness λ_s using the Lieberman sheath model [8]. If $\lambda_s < \Delta x$, then j_d is corrected. The revised value of j_d is then used to compute circuit parameters, among them the DC substrate bias.

The sheath potential and thickness from the HPEM are used with the Monte Carlo Sheath Transport module (MCST) of SPEEDIE to determine the ion velocity distribution (IVD). This module uses a hard ball collision model and a linear sheath field. It also considers the effect of pre-sheath ion heating on the IVD [9]. The IVD along with the fluxes of neutrals and ions from the HPEM are used in the 3-D Fluxes (3DF) module of the SPEEDIE to calculate local fluxes taking into consideration 3-D visibility along the two-dimensional cross section profiles of test structures. The surface kinetics (SK) model calculates local etch and deposition rates of the surface element and gives the etching rate of a material as a function of fluxes, ion energies, incident angles, and substrate temperature. The SK model used is a modification of the Langmuir limited adsorption model [4] to account for the effect of inhibitor deposition and its removal by ion bombardment on the effective ion flux [10,11]. The profile evolution module implements the surface movement caused by the etch and deposition rates from the SK The surface movement algorithm uses a new segment based geometric method, in which the conservation of material, or entropy condition, is obeyed. This is done by using the under and over lapping of the cells swept out by the initial movement of the segment to

determine the correct segment length and position. With this method there is no need for delooping. Re-emitted fluxes are used in the 3DF locally and in the HPEM.

3. Results

The complex simulator was tested in the case of polysilicon etching in a He/Cl_2 gas mixture. The process used in a commercially available RIE reactor was at 230 mTorr, power of 250 W, and gas flow of 75 and 150 sccm for Cl_2 and He, respectively. The following species were included in the HPEM: He, He*, He^+, Cl_2, Cl, Cl^+, Cl^-, e. The ion fluxes we quote (Fig. 3) are the sum of He^+, Cl_2^+, and Cl^+. Special overhang structures (Fig. 4) were used to extract surface parameters for the SK model and the angular spread of the IVD. The results (Fig. 5) show that the details of the experimental profile are well captured, and should be useful to predict evolution of other structures and the effects of process conditions on etch profiles.

4. Conclusions

Detailed modeling of etch profiles and studies of etch uniformities across the wafer can be obtained by using a profile simulator that takes into account reactor, plasma properties, etch chemistry, and surface kinetics effects. The feasibility of such an effort was proven in a case of a pure Cl_2/He gas mixture. Etching additives increase the complexity of computation but can be used if the proper chemical data are available.

5. Acknowledgment

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4. References

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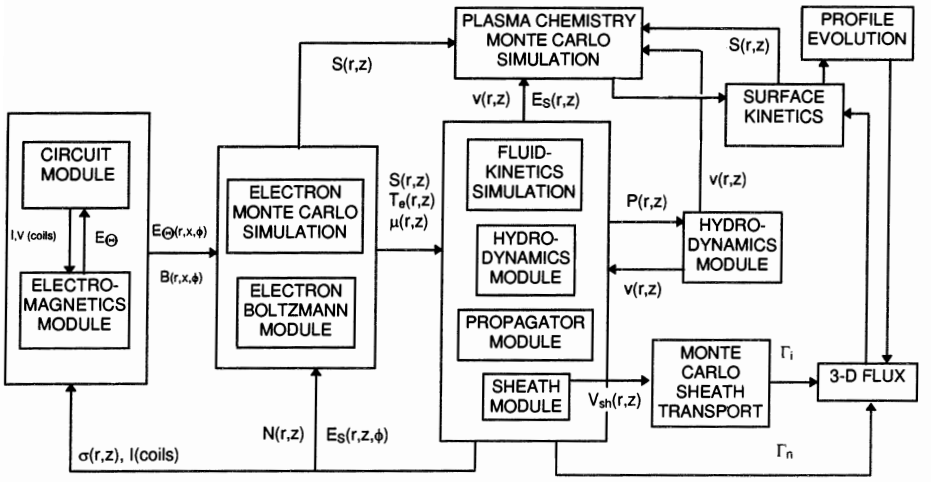


Fig. 1: Flow chart of the simulator, indicating equipment, plasma, chemistry, and profile evolution modules.

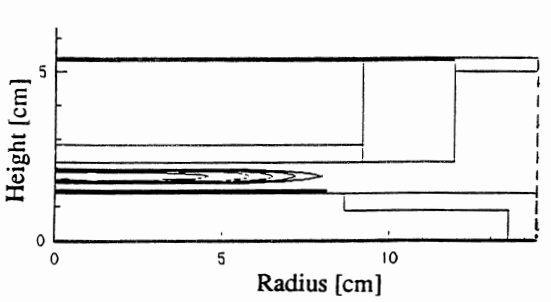


Fig. 2: Contour plot of total ion density in the reactor. maximum density is 5.5 e11 cm^{-3}.

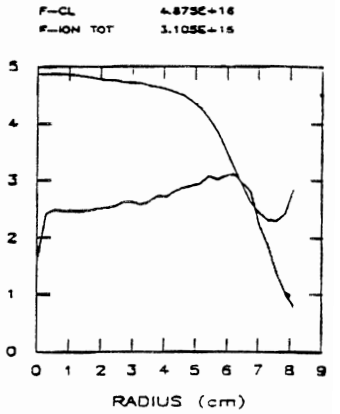
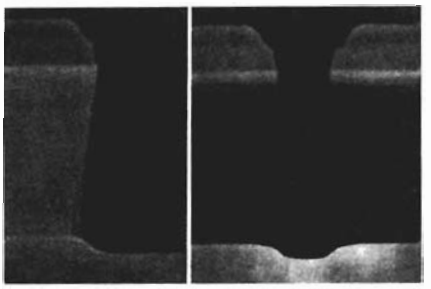
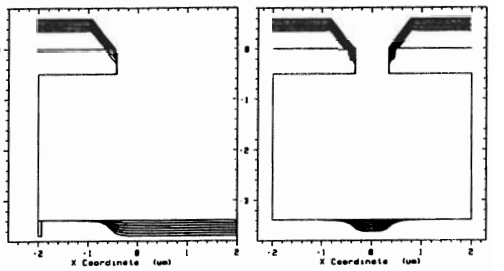


Fig. 3: Radial distribution of ion and Cl flux in the reactor.



(a) (b)

Fig. 4: SEM pictures of the overhang structures with wide opening (a) and narrow opening (b), used to determine the surface kinetics parameters.



(a) (b)

Fig. 5: Simulated profiles of the overhang structures form Figs. 4.