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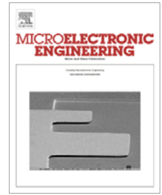

Integrated plasma processing simulation framework, linking tool scale plasma models with 2D feature scale etch simulator

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ABSTRACT

An integrated, extensible, full featured inductively coupled plasma (ICP) reactor simulation environment with a 2D feature scale etch simulator is presented. It incorporates tool scale plasma chemistry and feature scale trench evolution. Flexibility is achieved by software plugins for gas phase and surface reaction models that can be freely adapted and extended to a wide range of reactant-material systems. Available plasma chemistries cover SF_6, C_4F_8 and O_2 plasmas and are implemented by global models capturing both gas phase and wall-surface reaction kinetics. Surface reaction models for Si, SiO_2, and organic polymers have been developed. Validation of simulation agreement with experimental data is presented for etching of Si by SF_6 plasma.

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1. Introduction

In recent years significant progress in simulation of plasma reaction equipment and feature etching [1] was made. Due to complexity of physical effects and chemical processes, simulation software to date is limited to either tool size plasma simulations or feature size profile evolution. Joined simulators are few in number and are restricted to relatively large feature sizes. In this work we present a simulator which brings together (1) tool size gas phase and sheath models, (2) feature scale species transport modules, and (3) surface reaction modules.

2. Integrated trench etch simulation framework

To carry out trench etch simulations, a software framework with graphical user interface (GUI), script interpreter, and programming interface was developed. Flexibility and extensibility is obtained by a plug-in mechanism allowing introduction of new plasma and surface reaction models. Because of the integration of tool size and feature size models into the framework, the simulator accepts multiple process parameters, e.g. pressure, ICP power, temperature, etc.

3. Gas phase model and simulation

The gas phase is described by global-type models which couple gas phase and wall-surface reaction kinetics. The equations of the models are the mass balances of the species in the gas phase and on the wall-surface and the electron energy balance. They include electron impact reactions (ionizations, dissociations, attachments) as well as detachments and recombinations of charged and neutral species. The inputs of the models are the operational parameters (e.g. pressure, power) and the outputs are the densities of the species in the gas phase. Currently gas phase models for SF_6 [2], C_4F_8 [3] and O_2 plasmas are available and integrated into the reactor simulation. The densities of neutral species were measured by optical emission spectroscopy (OES) and electron density and temperature within the plasma measured by hairpin and Langmuir probes. They are available for the further validation of the gas phase models and the calculation of the coefficients of wall-surface reactions [2].

4. Transport of plasma species

Transport of species from plasma to sample surface at tool size is modeled by a simplified, extensible sheath model. Considering the ions within the plasma as an ideal gas, their velocities are Maxwell–Gaussian distributed. The components of their velocity vectors are therefore normal distributed with mean value of zero and independent of each other. It is assumed that the ions enter the sheath with thermal velocity vertically into the electric field whereas the floating potential is neglected. While the lateral velocity is unaltered by the sheath, the vertical velocity increases due to DC bias acceleration. As a consequence the angular distribution function IADF of ions predicted by the simplified sheath model is

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$$f(\varphi) = \frac{1}{\sigma_\varphi\sqrt{2\pi}} e^{\frac{-\varphi^2}{2\sigma_\varphi^2}}$$

with ion angle $\varphi = \arctan\left(\frac{v_{lat}}{v_{verti}}\right)$ and standard variance

$$\sigma_\varphi = \sqrt{\frac{k_{Boltz}T_i}{2eV_{DC}}}$$

With these approximations the ion energy distribution IEDF is a Gaussian distribution centered at

$$\mu = eV_{DC} \quad \text{and} \quad \sigma = \sqrt{\frac{k_{Boltz}T_i}{2eV_{DC}}}$$

The sheath model does not consider interactions of ions within the sheath and averages the effects of the alternating RF field. It is therefore reasonable for plasma conditions where the mean free path of ions is long, compared to the thickness of the sheath and on the other hand, the ions remain in the sheath for several periods of the RF field.

Within features, effects like shadowing, adsorption and resorption of species are considered using new transport models [4] and extensible surface reaction models for a wide range of material-species systems. Etching of Si, SiO_2 [5], and polymers such as poly (methyl methacrylate) (PMMA) as well as deposition of fluorocarbon polymer are covered. Reactant transport simulations include shadowing of ions and diffuse reflection of neutrals. Neutral transport is calculated by a finite element method similar to the radiosity method used in computer graphics [6]. Comparison of cross sectional profiles and etch and deposition rate measurements were obtained from experiments and compared to simulations to tune model parameters and validate correctness of models.

5. Etching of silicon by SF_6

The simulator has been used to model photoresist masked silicon etching by SF_6 plasma. The etch rate of photo resist is obtained from a linear model of weighted fluxes j_i of species ($SF_6, SF_5, SF_4, SF_3, F_2, F, SF_5^+, SF_4^+, SF_3^+, SF_6^-$, and F^-) from the plasma. Coefficients a_i are estimated from etch rate measurements of similar experiments and from literature [7]. The etch rate of photo resist is calculated by

$$ER_{PR} = \sum_{i \in Species} a_i j_i$$

For the etching of Si by SF_6 the surface processes are described by a Langmuir-type surface model which is based on surface site balances. The inputs of the surface model are the local fluxes j_i of the species i and the outputs are the etching rate ER_{Si} and the effective sticking coefficients $S_{E,i}$ of the species [8] on the etched surface. The central equation of the model is a surface site balance on Si at steady state

$$s_F(1-\theta_F)(p_1\, j_F) - 2\beta_F\theta_F(p_2\, j_{ion}) = 0$$

where θ_F is the proportion of surface coverage by fluorine, j_{ion} the summarized ion flux, and $s_F = 0.2$ is the sticking probability of fluorine on uncovered Si. The etch rate of Si is then calculated as the sum of pure chemical and ion enhanced etching of the fluorine covered surface

$$ER_{Si} = p_1\frac{k}{\rho_{Si}} j_F + p_2\frac{\beta_F}{\rho_{Si}} j_{ion}\theta_F$$

where

$$\beta_F = \begin{cases} b_{F,0}\left(\sqrt{E} - \sqrt{E_{th}}\right) & : E \geqslant E_{th} \\ 0 & : \text{otherwise} \end{cases}$$

with $k = 0.075$ and $b_{F,0} = 5\ eV^{-\frac{1}{2}}$ chemical and ion enhanced etch coefficients respectively, E the mean energy of ions, $E_{th} = 4$ eV the threshold energy for ion enhanced etching, and ρ_{Si} the Silicon atome density. The linear coefficients p_1 and p_2 were introduced to rescale the fluxes calculated by the gas phase model to the specific reactor.

The effective sticking coefficient for fluorine which loops back to the calculation of the fluorine flux is also calculated by the model as

$$S_{E,F} = s_F(1-\theta_F) + 4k$$

To obtain the relevant coefficients for surface reaction models, simulations were compared with experimental measurements as a function of feature size, bias, temperature, pressure, and gas flow (process parameter values shown in Table 1). Experimental samples were masked with long trench lines of photo resist of 1, 2, 5, 10, 20 μm width. The experiments were carried out on a prototype ICP reactor developed by Oxford Instruments Plasma Technology Ltd, (OIPT).

To separate pure chemical reactions from ion bombardment induced chemistry, etching profiles were characterized as a function of DC bias (0, 44, and 70 V). The DC bias in this context is the potential difference between the r.f. powered table and the grounded chamber walls. It was measured at the matching box. Experiments were compared to simulations, and fitting parameters were extracted to adjust simulations. Linear etch rate coefficients $p_1 = 0.8$ and $p_2 = 0.45$ for neutrals and ions were fitted to the specific reactor using a single experiment and were fixed for the rest of simulations. Sticking coefficients for neutral species were obtained from literature [9]. Since the gas phase model was already validated using plasma diagnostics, no additional parameter fitting was performed. Fig. 1 shows a cross section of an isotropic etching experiment overlaid by a profile obtained from simulation using the same process parameters. Depth, undercut and profile shape are in good agreement between experiment and simulation.

Fig. 2 compares the ratio of profile undercut to etching depth for the experiments and simulations as a function of trench width and DC bias. The experimental data reveals a trend towards more undercut (higher undercut:depth ratio) for decreasing DC bias.

Table 1
Process parameters of etch experiments.

Parameter	Value
Feature size	1, 2, 5, 10, 20 (μm)
DC bias	0...84 (V)
Pressure	8.1, 10, 25 (mTorr)
ICP power	1000 (W)
SF_6 flow	25, 50 (sccm)

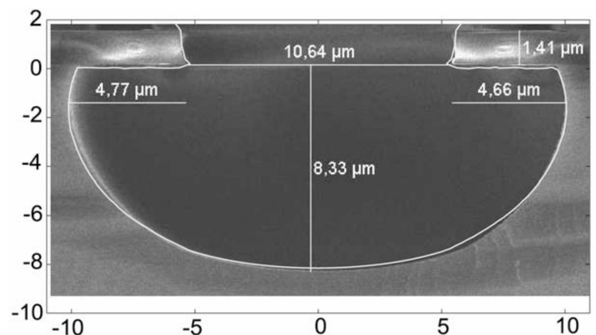

Fig. 1. Cross section of experiment and overlaid simulation profile etched for 60 s with 50 sccm SF_6 at 70 V DC bias, 25 mTorr pressure, and 1000 W ICP power.

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