A PLASMA CHEMISTRY MONTE CARLO MODEL FOR
ION AND RADICAL FLUXES AND ENERGY DISTRIBUTIONS
IN INDUCTIVELY COUPLED PLASMA ETCHING REACTORS

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In the low pressure, high density, inductively coupled plasma etching reactors
being currently developed, the fluxes and energy distributions due to ions and neutral
radicals need to be examined. This information can be used to determine the etch rate,
anisotropy, and uniformity over large wafers for a wide range of power, pressure, and
substrate rf bias. This will allow further development towards faster processing and
better yields. A Plasma Chemistry Monte Carlo model has been developed to
theoretically examine etching for new reactor designs over their full range of input
parameters. A companion 2 dimensional hybrid fluid-kinetics model produces spatially
dependent sourcing of plasma species, time dependent electric fields, and advective flow
velocities of the gas which are used by the Plasma Chemistry Monte Carlo model. The
model follows the paths of ion and neutral radical pseudoparticles in the reactor.
Statistics are collected at the reactor surfaces as well as within the gas. From these
statistics, the fluxes, angular distributions, and energy distributions of the particles hitting
the wafer can be determined. In the reactor, the spatial distribution of momentum flux,
temperature, and density for all plasma species is also calculated.

Results are presented here for a 70/30 gas mixture of Ar/Cl₂ parameterized over
power, pressure, and substrate rf bias as well as changes in the inductive power coil
configuration. For a pure Ar plasma, the effects of the addition of a dielectric ring under
the wafer are also examined. The fluxes and angular distributions are used to calculate
etch rates as well as etch uniformity for the Ar/Cl₂ plasma based on Dane and Mantei’s
etching model for Cl₂ etching of Si.
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I. INTRODUCTION

The use of plasma reactors for semiconductor manufacturing is becoming predominate in industry due to their capability for producing very small dimension, low damage features. To produce the smaller dimensions on larger wafers required in future markets, reactors are necessary which can produce highly anisotropic etching with little damage and good uniformity over large areas. Inductively coupled plasma (ICP) reactors are being developed to meet these requirements.

One ICP reactor design uses the “stove-top” coil configuration in which the powered coils are spiral in shape and are placed on top of the cylindrical reactor. These reactors have produced high plasma densities ($10^{11}$-$10^{12}$ $\text{cm}^{-3}$) at low pressures which allow fast, highly anisotropic etching. Low pressures give more anisotropic ion bombardment. However, higher plasma densities are required to sustain reasonable etch rates. Keller et al. have experimentally demonstrated that ion densities in these reactors are linearly proportional to input inductive power. The addition of a separately controlled radio frequency bias on the substrate also allows semi-independent control of the average ion impact energy. For substrate bias powers less than 30% that of the coil power, the sheath potential can be considered to be independently controlled by the bias amplitude.

Etching performance of these reactors is primarily dependent on the energy distribution, angular distribution, and magnitude of fluxes of the ions and radicals as well as their respective uniformities over the wafer surface. Most current surface models for etching have a dependence on at least the ion and radical fluxes and the average ion impact energy.$^{3,5}$ Most etching models include as their primary etching mechanism ion enhanced chemical etching. In this process, radicals bond to wafer surface atoms and partially saturate the surface. Ion impacts then provide the necessary energy to push the molecule off the surface.

Ion energy distributions (IEDs) can be affected by many factors in these reactors. Due to the very thin sheaths produced in these low pressure, high density systems, ion transit times can be a fraction of the substrate bias cycle time. These ions will feel the instantaneous sheath potential rather than the time averaged potential. This produces
IEDs which are broadened into a bimodal shape, as seen in conventional capacitively coupled RIE reactors at low frequencies or with light ions.\textsuperscript{6} In these reactors, the difference between energy peaks in the IEDs has been shown to vary inversely with the square root of ion mass. An ion energy distribution which is spread over a wide range of energies (10s of eV) could change etching characteristics as compared to a narrow IED. This results from the fact that higher energy ions can penetrate more deeply, creating more damage and thicker mixing layers, whereas lower energy ions could be below some cutoff energy, thereby causing no etch. Additionally, hot neutrals produced by the charge exchange between neutrals and fast-moving positive ions have energies commensurate with the ions and could impact with enough energy on the wafer to enhance chemical etching. As shown by the modeling of Maneshijn and Goedheer,\textsuperscript{7} these “hot” neutrals can have very broad energy distributions as compared to the ions. These fast charge exchange reactions also deplete energy from the ions by converting neutrals to slow ions.

Reactor geometry can also play a large role in etching. Changes in the coil placement and shape have been studied both through experiments\textsuperscript{8} and modeling\textsuperscript{9} and have been shown to be one of the strongest factors in plasma density and uniformity. By changing the system boundary conditions, surface topography as well as the profile of structures that are in contact with the plasma can affect the uniformity and “quality” of etching.\textsuperscript{10,11} Also, structures below the wafer surface, such as dielectric materials used for electrostatic chucks, can act as capacitors in series with the sheath and wafer capacitances over which the substrate bias potential is dropped and, therefore, affect the local impedance. For nonconductive wafers, this can strongly affect the local shape of the sheath as well as its potential.\textsuperscript{12}

Variations in the ion angular distribution (IAD) can also affect the etch characteristics. As mentioned before, very anisotropic etching is required, which means that the ions must impact at very small normal angles. Changes in reactor parameters, such as substrate bias or reactor geometry, could lead to changes in the IAD and, therefore, the etching profile. By changing the shape of the sheath, subwafer structures can also perturb the local IAD.

There have been previous studies\textsuperscript{7,13-16} of these IEDs for pure gases. However, studies of multicomponent gases have been limited. Hwang and Kushner\textsuperscript{17} have modeled
the effect on the shape of the IED of more complex chemistries (He/N₂ and He/CF₄/H₂), which include nonsymmetric charge exchange and endothermic processes. In this work, a plasma chemistry Monte Carlo simulation (PCMCS) has been developed to further study the IEDs, IADs, and fluxes of both ions and radicals on the wafer. Using data produced by the hybrid plasma equipment model (HPEM), such as plasma species sources and time dependent electric fields, the PCMCS generates statistics for the impact of ions and radicals on all surfaces of the reactor as well as densities and momentum fluxes of the particles within the plasma. These statistics can then be used with surface chemistry models to estimate etching rates and uniformity.

In Chapter II, the computational model is described in detail. Results of the simulation for pure Ar and Ar/Cl₂ chemistries as a function of power, pressure, bias, and reactor geometry are presented in Chapter III. A generic LAM 9x00 reactor was used as the basis for the simulated reactor geometry for which inductive powers ranged over 150-1000 W, pressures ranged over 5 to 20 mTorr, and substrate biases ranged over 0-150 V. For high inductive powers and high pressures, the sheath thickness is thin enough to produce very broadened IEDs whose widths vary linearly with substrate rf bias amplitude. Etch rates are strongly enhanced by increases in power due to increased fluxes of all species on the wafer. However, increases in rf bias amplitude have little effect on etch rates, since the reactor parameters are within the neutral starved regime for most cases. Increases in pressure cause the system to transition from a neutral starved to an ion power flux starved regime. Ion and radical fluxed, energy distribution, and angular distributions are studied for all cases, as well as their effects on the etching of the wafer.
II. MODEL DESCRIPTION

The model of low pressure, high density plasma reactors consists of a two-dimensional (2D) hybrid model, as flowcharted in Figure 1, (all figures and tables appear at end of thesis) which is composed of an electromagnetic module (EMM), an electron Monte Carlo simulation (EMCS), a fluid-chemical kinetics simulation (FKS), and a hydrodynamic advective flow module (HAFM). An offline plasma chemistry Monte Carlo simulation uses data calculated by the 2D hybrid model to resolve energy distributions and fluxes of species in the reactor and on the reactor surfaces. These results are the focus of this paper. The PCMCS simulations were run on a VAX Alpha 3000/600 and took 20 to 30 hours to complete 20 iterations for statistically smooth results.

A. 2D Hybrid Modules

The electromagnetic module calculates the electric and magnetic fields, \(E(r,z,\phi)\) and \(B(r,z,\phi)\), in the entire volume by direct solution of Maxwell’s equations and is more fully described in Ref. 18. The electric field is found by successive-over-relaxation solution of

\[
\nabla \cdot \frac{1}{\mu} \nabla E = \frac{\varepsilon^2 (\varepsilon E)}{\partial z^2} + \frac{\partial (\sigma E + J_0)}{\partial t}, \quad (\text{II.i})
\]

where \(J_0\) is the driven coil currents, currents, and fields are assumed to be harmonic, and plasma conductivity is calculated as

\[
\sigma(r) = \sum_i \frac{q^2 n_i(r)}{m_i} \frac{1}{\nu_{mi} + i\omega}, \quad (\text{II.ii})
\]

where the sum is over all charged species.

The electron Monte Carlo module follows electron trajectories using the azimuthal electric and magnetic fields, \(E(r,z,\phi)\) and \(B_\theta(r,z,\phi)\), from the EMM, and the
electrostatic fields $E_s(r,z,\phi)$ calculated by the FKS. Prior to simulation, the probability arrays for all pertinent electron impact collisions with the gas species (e.g., elastic, excitation, and ionization) are calculated from the collision frequencies

$$v_{ij} = \left( \frac{2e_i}{m_e} \right)^{1/2} \sigma_{ij} N_j,$$  \hspace{1cm} (II.iii)

where $\sigma_{ij}$ is the electron impact cross section at energy $i$ for process $j$, and $N_j$ is the density of the collision partner for process $j$. The probability arrays incorporate a null collision frequency using the maximum collision frequencies. Electron trajectories are initialized randomly from a Maxwellian distribution and are distributed in the reactor based on a weighting by the plasma density distribution. The electrons’ trajectories are advanced using the electric and magnetic fields from the EMM as well as the time-varying electrostatic field $E_s(r,z,\phi)$ from the FKS on successive iterations. Species densities are calculated in the FKS from the previous iteration. After ~20-50 rf cycles, electron impact source functions are calculated from the time-averaged electron energy distribution $f(\epsilon,r,z)$ to be used in the FKS.

$$S_{ij}(r,z) = n_e(r,z)\delta_{ij} N_{ij}(r,z) \int_0^\infty f(\epsilon,r,z) \times \left( \frac{2e}{m_e} \right)^{1/2} \epsilon^{1/2} \sigma_{ij}(\epsilon) d\epsilon,$$  \hspace{1cm} (II.iv)

where $n_e$ is the electron density, $\delta_{ij}$ is $\pm 1$ if process $j$ is a source or loss of species $i$, and $N_{ij}$ is the density of the collision partner. The mechanics of this module are more fully described in Ref. 18.

The fluid-chemical kinetics module solves the continuity equation for all species as well as Poisson’s equation.

$$\frac{\partial N_j}{\partial t} = \nabla \cdot \left( \mu_j q_j N_j E_z - D_j \nabla N_j \right) + \left( \frac{\partial N_j}{\partial t} \right)_e,$$  \hspace{1cm} (II.v)
and

$$\nabla \cdot \mathbf{E_s} = -\nabla^2 \Phi = \frac{\rho}{\varepsilon_0} . \quad \text{(II.vi)}$$

The symbols $\mu_j$, $D_j$, and $q_j$ are respectively the mobility, the diffusion coefficient, and the charge of species $j$, while $\rho$ is the charge density. Also in the formulae above, $\mathbf{E_s}$ is the electrostatic field and $\Phi$ is the electrostatic potential. Finally, $(\partial N_j/\partial t)_e$ is the change in density due to all collisions and contains effects due to heavy particle collisions as well as the electron impact source function $S_j(r,z)$. To bypass the limits of the dielectric relaxation time,

$$\Delta t_d = \min \left( \frac{\Delta r}{\mu_j E_r}, \frac{\Delta z}{\mu_j E_z} \right) , \quad \text{(II.vii)}$$

which can cause unstable oscillations in the charge density for time steps larger than $\Delta t_d$, a semi-implicit scheme is used to update the potential to $t+\Delta t$,

$$\nabla \cdot \varepsilon \nabla \Phi(t + \Delta t) = -\frac{1}{\varepsilon_0} \left[ \rho(t) + \Delta t \frac{\partial \rho}{\partial t}(t) \right] , \quad \text{(II.viii)}$$

where

$$\frac{d\rho}{dt} = \sum_i e q_i [\nabla (D V N_i + q_i N_i \mu_i \nabla \Phi)] . \quad \text{(II.ix)}$$

Radio frequency capacitive bias of the substrate is allowed by imposing a sinusoidal potential on specified materials in the reactor. Also, capacitive coupling of the radio frequency biased substrate is included by the use of a circuit model of a capacitor in series with the radio frequency source. This model is more fully explained in Ref. 18.
The hydrodynamic advective flow model is based on the solution of Navier-Stokes fully compressible equations,

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 ,
\]  

(II.xa)

\[
\frac{\partial (\rho \mathbf{v})}{\partial t} = -\nabla P - \nabla (\rho \mathbf{v} \cdot \mathbf{v}) - \nabla \cdot \mathbf{F} ,
\]  

(II.xb)

and

\[
\frac{\partial (\rho c_v T)}{\partial t} = H_J + \nabla \cdot \kappa \nabla T - \nabla \cdot (\rho c_v T \mathbf{v}) - P \nabla \cdot \mathbf{v} + \Gamma ,
\]  

(II.xc)

where \( \rho \) is the mass density, \( P \) is the thermodynamic pressure, \( \tau \) is the viscosity tensor, \( H_J \) is the Joule heating from the plasma, \( \kappa \) is the thermal conductivity, and \( \Gamma \) is the dissipative heating term. Slip boundary conditions were used to account for long mean free path transport. The model is more fully described in Ref. 18 and follows the ideas presented by Thompson.19 See Figure 2 for an example of the advective flow through the reactor where there are high flow rates at the inlet and outlet, but stagnation near the center.

**B. Plasma Chemistry Monte Carlo Model**

The Plasma Chemistry Monte Carlo model was developed to examine plasma species, including neutrals, ions, and excited state species, as they transport in the plasma and impinge on the reactor surfaces. The PCMCS model uses 2D electron impact source functions for charged, neutral, and excited species from the EMCS, the time-dependent electrostatic fields \( E_s(r,z,t) \) from the FKS, and the advective flow fields \( v_r(r,z) \) and \( v_z(r,z) \) from the HAFM. From this data, pseudoparticles are released in the reactor, and location-dependent angular and energy distributions as well as fluxes are found for all plasma species at the reactor surfaces. Also, densities as well as momentum fluxes in the plasma are calculated. The Monte Carlo simulation is iterated ten to twenty times, which
allows plasma species densities and feedstock gas depletions to be calculated. The revised densities are used in the following iterations for collisions between Monte Carlo species and adjustment to feedstock densities.

i. Mesh generation

A material-mesh definer (MMD) has been developed to describe the reactor geometry and is used by all modules in the model. The mesh consists of a rectilinear grid on which are defined the material properties to produce the desired reactor geometry. The produced arrays define the boundary locations and orientations between materials as well as information such as the conductivity of each material. This allows the properties of the plasma, such as electric fields, densities, and species sourcing, to be defined on the same grid within each module. As shown in Figure 3, the fields’ points are located on the cell boundaries, which allows boundary conditions to be set normally to material-material boundaries, whereas densities are calculated at cell centers, which allows for cell averaged densities.

ii. Particle motion

The particles are produced, according to the source functions passed from the FKS, with a random thermal velocity and direction which will be described in more detail in Section II.B.iii. The acceleration of each charged particle is determined by the electric fields $E_r(r,z,t)$ and $E_z(r,z,t)$. The acceleration of the particle is derived from linear interpolation between the four field points surrounding the cell.

A time of flight is calculated as

$$\Delta t_{\min} = \min(\Delta t_{\Delta r}, \Delta t_{\Delta z}, \Delta t_{\text{col}}),$$

(II.xi)
where $\Delta t_r$ and $\Delta t_z$ are the times to move a fraction of $\Delta r$ or $\Delta z$ (cell width) and $\Delta t_{col}$ is the time to the next collision. The time for transition of one cell width is determined by solving the equation of motion for $\Delta t$. The time to the next collision is

$$\Delta t_{col} = r\left(\sum_k v_{col,k}\right)^{-1}, \quad (\text{II.xii})$$

where $v_{col,k}$ is the collision frequency for process $k$ and $r$ is a random number between zero and one.

A particle can also collide with a surface. When a particle is moved, it can transition from a gas cell to a solid cell. In this case, the particle is moved to a position just inside the gas cell, and a surface reaction is determined as described in Section II.B.v. A flowchart portraying pseudoparticle motion is shown in Figure 4.

**iii. Particle initialization**

Particles are launched in the reactor according to the spatial distribution of the source functions $S_j(r,z)$ obtained from the EMCS. The number of particles of species $j$ released in a given cell is based on the spatial distribution of the source function and the maximum number of particles allowed,

$$NumS_j(r,z) = \max\left\{NumS_{\text{min}}, NumPart \times \frac{S_j(r,z)V(r,z)}{NumS_{\text{total}}} \times \frac{1}{SWt_i(r,z)}\right\}, \quad (\text{II.xiii})$$

where $NumS_{\text{min}}$ is the minimum allowable number of particles released in a cell for each species, $NumPart$ is the total number of particles released, and $V(r,z)$ is the volume of the cell.

$$NumS_{\text{total}} = \sum_{i,r,z} S_i(r,z)V(r,z)SWt_i(r,z), \quad (\text{II.xiv})$$
gives the total weighted sum of the sources, and

\[ SW_{t_i}(r, z) = \frac{\log[S_i(r, z)]}{\log[S_{max}]} , \]  

(II.xv)

where

\[ S_{max} = \max_{r, z} [S_i(r, z)] . \]  

(II.xvi)

Using this logarithmic weighting allows for a statistically significant number of particles to be released in low source cells. The actual particle weighting (#molecules/sec) is then

\[ W_{t_i}(r, z) = S_i(r, z)V(r, z) / NumS_i(r, z) . \]  

(II.xvii)

Density statistics for the Monte Carlo species are determined by adding the weighting \( W_{t_i} \) times the transit time through the cell to give the pseudoparticle’s contribution to that cell. After successive iterations, depletions of feedstock gases are calculated and adjustments are made to densities and weights by the factor \((1-%_{\text{depleted}})\) for “daughter” species as well as the feedstocks. Back averaging of the depletion values is used to speed convergence. The fraction of the last value averaged in is generally ~0.3. This depletion value is allowed to converge in the first few iterations. For negative values of \( S_i(r, z) \) or loss regions for species \( i \), reactions are created based on collisions with a dummy species which removes particles at the rate specified by \( S_i(r, z) \).

Each particle is released with a random direction, position in the cell, and speed chosen from a Maxwellian distribution,

\[ v = \left( \frac{8}{\pi} \frac{k_b T}{m_j} \ln \left( \frac{1}{(1-r)^2} \right) \right)^{1/2} , \]  

(II.xviii)
where \( k_B \) is Boltzmann’s constant, \( T \) is the temperature of the gas, \( m_j \) is the mass of species \( j \), and \( r \) is a random number between zero and one. In general, the temperature used is around 300\(^\circ\)K, or room temperature. The “bath” or fluid velocity at that cell, which came from the hydrodynamic advective flow module, is added to the thermal velocity, allowing the Monte Carlo particles to “see” the advective flow.

**iv. Gas phase reactions**

Several types of gas phase reactions are included for the Monte Carlo particles, such as elastic, charge exchange, three body association, as well as any other two body reactions appropriate to the chemistry. Probability arrays for collision frequencies of each species are calculated using the reaction coefficients \( k_j \) and maximum collision partner densities \( N_{i,\text{max}} \),

\[
P_j = \sum_{i=1}^{j} k_j N_{i,\text{max}}.
\]  

(II.xix)

However, for three body reactions, the density of the third body must be added, in this case the total gas density \( N_{\text{total}} \),

\[
P_j = \sum_{i=1}^{j} k_j N_{i,\text{max}} N_{\text{total}}.
\]  

(II.xx)

A time to next collision for each particle is calculated as \( \tau = \nu_{\text{total}}^{-1} \ln(r) \), where \( \nu_{\text{total}} \) is the total collision frequency for all processes possible for that species and \( r \) is a random number. The process which has occurred is found by indexing the probability matrix for that species with a random number \( r \), where \( P_{i-1} < r \leq P_i \) indicates that process \( i \) has occurred. The actual occurrence of a reaction is then found by

\[
r \leq \frac{N_i(r, z)}{N_{i,\text{max}}},
\]  

(II.xxx)
where $r$ is a random number between zero and one. This allows for null collisions where the collision partner density is below its spatial maximum. When feedstock species or other non-MC species are created by the reaction, the particle is removed. If, however, one or two MC species are produced, the colliding particle’s identity is changed and a new MC particle can be added. See Tables 2 and 3 for the reaction schemes used in the simulations.

The elastic collisions between feedstock species and Monte Carlo particles allow the particles to sense the density and, therefore, the mean free path $\lambda_{mfp}$ as well as the advective flow of the gas through the system. The rate coefficients for elastic collisions are calculated using Leonard-Jones radii to simulate hard sphere collisions,

$$k_i = v_{\text{thermal}} \rho \left(\frac{\sigma_1 + \sigma_2}{2}\right)^2,$$  

(II.xxii)

where $v_{\text{thermal}}$ is the thermal velocity of the species and $\sigma_k$ is the Leonard-Jones radii for species $k$. Lennard-Jones parameters were obtained from R. A. Sveha, NASA Technical Report No. R-132, 1962. In a collision, the mesh particle that has been collided with is given a velocity which is the sum of a random thermal (Maxwellian) velocity, as described earlier, and the advective flow velocity at that mesh point. In this way, through an energy conservative collision, the MC particle “feels” the effects of the advective flow. The energy gained or lost by the particle is derived by calculating a random scattering angle,

$$\theta_s = 2 \sin \left[r \cdot \min \left(\frac{m_{cp}}{m_i} , 1 \right)\right],$$  

(II.xxiii)

where $r$ is a random number (0,1), $m_{cp}$ is the mass of the collision partner, and $m_i$ is the mass of the particle. For cases in which the particle energy is greater than that of the collision partner, the energy loss is
\[ \Delta E = -E_i \left[ 1 - \cos(\theta_i) \right] \frac{m_r}{2m}, \]  

(II.xxiv)

while for cases where the particle energy is less than that of the collision partner, the energy gain is

\[ \Delta E = E_{cp} \left[ 1 - \cos(\theta_i) \right] \frac{m_r}{2m}, \]  

(II.xxv)

where \( E_i \) is the energy of the particle, \( E_{cp} \) is the energy of the collision partner, \( m_r \) is the reduced mass, and \( m \) is the average mass.

Charge exchange reactions, including both symmetric and unsymmetric, such as,

\[ Ar(cold) + Ar^+(hot) \rightarrow Ar^+(cold) + Ar(hot), \]  

(II.xxvi)

and

\[ Cl_2(cold) + Ar^+(hot) \rightarrow Cl^+_2(cold) + Ar(hot), \]  

(II.xxvii)

are included since they can produce high energy (10’s of eV) neutral species in the plasma. In a charge exchange collision between a neutral and a positive ion, there is very little energy transfer, but the charged particle is neutralized while retaining its energy. For positive ion species such as \( Ar^+ \) in an argon plasma, this charge exchange rate can be high enough to allow hot neutral densities in the reactor to rival those of the corresponding ions. These high energy fluxes of neutrals to the substrate could play an important role in surface chemistry and, therefore, etch and deposition rates.

v. Surface reactions
Surface reactions are carried out on the basis of two parameters, a reflection coefficient and a reactive sticking coefficient, both of which range from zero to one. When a particle collides with a reactor surface including the substrate, a randomly generated number is compared to the reflection coefficient. If the random number is smaller, the particle is reflected with no change in identity. If the random number is greater, another random number is generated and compared to the reactive sticking coefficient. A number larger than the sticking coefficient corresponds to the particle sticking to the surface without production of gas species. However, if the number is smaller, a gas species particle is produced based on the surface reaction that has occurred. These coefficients can be dependent on the surface material, mainly with respect to the differences in the wafer and reactor wall materials.

The reactive sticking coefficient serves several purposes. In all cases, ions are considered to be neutralized at surfaces with a small probability of sticking. Excited states species are also returned as ground state products. Other species, such as the Cl radical, can be allowed to return as etch products. In the cases run, the chlorine radical was allowed to stick to nonreactive surfaces with 0.005 probability, producing the recombination product Cl$_2$ 50% of the time. For the reactive silicon wafer surface, the Cl reactively sticks with probability 0.05 and produces SiCl$_2$ 25% of the time, since the Cl coverage should be in steady state. This, in effect, allows for macroloading of the plasma system by these etch products as found in experiments.

In all cases, the particles are returned to the gas with an angle based on a modified cosine or Lambertian distribution,

\[
\Phi = \cos^{-1} \left[ \left( 1 - r \alpha \right)^{\frac{1}{(\beta + 1)}} \right], \quad (\text{II.xxviii})
\]

in which $r$ is a randomly generated number between zero and one, $\alpha$ is given by

\[
\alpha = -\cos \left[ \frac{\theta_{\max}}{180^\circ} \right]^{\beta + 1} , \quad (\text{II.xxix})
\]
β is the exponential cosine factor, and θ_{max} is the maximum normal angle which the particle can have. They are returned to the plasma with an energy chosen randomly from a Maxwellian distribution with temperature equal to that of the surface. Particles can also be allowed to return with a fraction of their prior energy, which allows for spectral scattering from the surface.

The etch model of Dane and Mantei\(^3\) for a chlorine plasma was used to calculate etch rates at the wafer and production rates of gaseous etch products. The etch model is based on a surface reaction scheme,

\[
Cl(g) + Si(s) \rightarrow SiCl(ads) ,
\]

and

\[
SiCl(ads) + SiCl(ads) + I^+ \rightarrow SiCl_2(g) + Si(s) .
\]

The \(SiCl(ads)\) is Cl bonded to a Si on the wafer surface, and \(I^+\) is any species of ion sticking the surface. This produces an etch rate formula which has a parallel resistive or series capacitive form,

\[
ER = \left( \frac{1}{\alpha \Gamma_{Cl}} + \frac{1}{\beta [J_i V_s - (J V)_{th}]} \right)^{-1} ,
\]

where \(\alpha = 2300 \text{ Å min}^{-1} \text{ mTorr}^{-1/2}\), \(\beta = 23 \text{ Å min}^{-1} \text{ mW}^{-1} \text{ cm}^2\) are fitting parameters, \((J V)_{th} = 85 \text{ mW cm}^{-2}\) is the threshold power flux to the wafer for the onset of etching, \(\Gamma_{Cl}\) is the Cl radical flux rate, and \(J_i V_s\) is the actual power flux to the wafer which was approximated by Dane and Mantei as the ion current density to the wafer multiplied by the sheath voltage. Dane and Mantei were unable to measure \(\Gamma_{Cl}\) in their experimental setup and, therefore, used an approximation of \(\Gamma_{Cl} \propto \sqrt{P_{Cl}_2}\) due to the \(Cl_2\) dissociation producing two Cl radicals. Therefore, their \(\Gamma_{Cl}\) is expressed in terms of \(\text{mTorr}^{-1/2}\) and the \(\alpha\) parameter has units of \((\text{Å min}^{-1} \text{ mTorr}^{-1/2})\). For these simulations, actual Cl radical fluxes in terms of \((\#_{Cl} \text{ cm}^{-2} \text{ s}^{-1})\) were calculated. Dane and Mantei’s \(\alpha\) parameter was
converted to units of (Å min$^{-1}$ cm$^2$ s) by calculating an estimated $\Gamma_{\text{Cl}}$ in terms of (#Cl cm$^{-2}$ s$^{-1}$). Based on a temperature of 600$^\circ$K,

$$\left| v_{th,z} \right| = \sqrt{\frac{2 k_b T}{\pi m_{Cl}}} \approx 2.98 \times 10^5 \text{ cm/s} \ .$$ \hspace{1cm} (II.xxxiii)

Using an estimated 50% dissociation of the Cl$_2$ at 1 mTorr gives a Cl radical density of $\sim 2.36 \times 10^{13}$ (#Cl/cm$^3$). The Cl radical flux to the wafer can be then estimated as

$$\Gamma_{\text{Cl}} \approx \frac{1}{2} N_{\text{Cl}} \left| v_{th,z} \right| = 3.5 \times 10^{17} \text{ cm}^{-2} \text{ s}^{-1} \ \{ \text{at 1 mTorr} \} \ .$$ \hspace{1cm} (II.xxxiv)

Using this estimated value for $\Gamma_{\text{Cl}}$, a new $\alpha$ can be found of $6.54 \times 10^{-15}$ (Å min$^{-1}$ cm$^2$ s). This is an upper limit estimate, since it does not account for spatial nonuniformity of the Cl and the effects of macroloading at the wafer. This etch model was used to look at radial uniformity of etch rates as well as the effects of varying inductive power, substrate rf bias, and pressure.

vi. Sheath thickness

In the 2D hybrid model as well as the PCMCS, the mesh size is generally much larger than the thickness of the sheath over the wafer for these high density plasmas (5 mm vs. 0.5 mm) especially for high inductive power cases (1 kW). In the PCMCS, Lieberman’s analytic model of a collisional, capacitive RF sheath$^{21}$ has been used to calculate the actual sheath thickness,

$$s = \frac{J_0}{e \omega n_0} \ ,$$ \hspace{1cm} (II.xxxv)
where $\bar{J}_0$ is the displacement current amplitude at the sheath edge, $\omega$ is the frequency (13.56 MHz), and $n_0$ is the plasma density at the sheath edge. Since the displacement current $J_{D0}$ calculated in the FKS is based on the original sheath thickness $s_0$, and $J_D$ varies linearly with the sheath thickness (assuming sheath capacitance varies linearly with thickness),

$$\bar{s} = \sqrt{\frac{J_{D0}}{e\omega n_0 s_0}}.$$  

(II.xxxvi)

To approximate the actual sheath thickness, the width in the $z$ dimension of the mesh cell above the wafer is set to the Lieberman model thickness. To maintain the original potential drop across the sheath, the accelerations of the charged particles in the sheath are multiplied by $s_0/s$.

vii. Collected statistics

A myriad of statistics are determined during the simulation, both in the plasma and at the surfaces which allow analysis of the system “unhindered” by the problems of physical experimental measurement. In the plasma, spatial and species dependent statistics are found for the radial and axial momentum flux, the kinetic energy, the temperature, and the density. At the surfaces, spatial and species dependent statistics are found for angular distribution, flux, and energy distribution of particles. These statistics can be viewed graphically in two or three dimensions to help explain the effects of changes in the reactor parameters such as pressure, power, or reactor geometry.
III. RESULTS AND DISCUSSION

In this section, the results of the cases run as listed in Table 1 are shown and described. The Ar/Cl₂ (70/30) chemistry has been parameterized over gas pressure, inductive power, and substrate rf bias as well as changes in the coil configuration. A pure argon plasma was used for the subwafer dielectric cases, and a pure chlorine plasma was used for the cases compared to the LAM etching data. In all cases, the frequency for both the inductive coils and the substrate rf bias was 13.56 MHz and the flow rate through the reactor was 80 sccm. The gas and surface phase chemical reactions for all chemistries are listed in Tables 2 and 3. The reactor geometry used is based on a generic LAM 9x00 TCP reactor with pressures in the range of 5 to 20 mTorr, powers of 150 to 1000 W, and substrate biases of 0 to 150 V. Typical conditions are more completely described below, and a schematic of the reactor is shown in Figure 5.

A. Canonical Cases

The canonical cases are an Ar/Cl₂ (70/30) gas mixture at 10 mTorr and 500 W ICP power with a gas flow of 80 sccm and with or without a rf bias on the substrate of 100 V. As shown in Figure 6, the power deposition for the case is a maximum of 1.8 W/cm³ and is concentrated only 1-2 cm below the quartz window. This is due to field penetration from the coils being limited by the conductivity and, therefore, the skin depth of the plasma. The ion density has a maximum of $1.3 \times 10^{12}$ cm⁻³ at ~7 cm (centered under the coils) and ~3 cm below the quartz window. The ion has a diffusive profile going to the surfaces of the reactor, as is shown in Figure 7(a), which shows the main ion density contributor Cl₂⁺. The main radical or neutral density is due to Cl, which has a maximum of $3.65 \times 10^{13}$ cm⁻³ near the center of the reactor and drops off radially. This distribution is due to sourcing near the top center of the reactor, with a gas flow inward at the top and outward at the bottom and stagnation near the center, as is shown in Figure 7.

The fluxes of the ions and neutrals to the wafer surface are very uniform, as shown in Figure 8. The ions are sourced well above the wafer and diffuse to an almost uniform density over the wafer. The density distribution of the Cl radical is diffusion
dominated and, combined with a low sticking coefficient at the walls, leads to high radial uniformity. There is a slight rise at the center of the ion distribution since it is closest to the density maximum. Over 70% of the flux is due to $\text{Cl}_2^+$, since the electron impact ionization of Cl$_2$ is several times faster than that of Ar and Cl$_2^+$ is produced in the nonsymmetric charge exchange of Cl$_2$ with Ar$^+$ and Cl$^+$.

The neutrals impact the wafer with a nearly Maxwellian velocity distribution with temperature of 600-700°K, as shown in Figure 9(a). In this gas mixture, however, hot neutrals can be formed by charge exchange. The fastest process is the symmetric charge exchange for Ar, since the density of the feedstock argon is the largest. This produces hot Ar with broad energy distributions at the wafer reaching as high as 20-30 eV and fluxes of $3 \times 10^{17}$ cm$^{-2}$s$^{-1}$, as shown in Figures 9(b) and (c). This corresponds to power fluxes to the wafer $\sim 20$ mW/cm$^2$, which could play a role in supplying energy for etching processes.

For the unbiased case, the ions impact the wafer with a single peaked distribution shifted by the self-bias potential of the sheath, in this case $\sim 6$ eV, as shown in Figure 10(a). The ions in the reactor with the 100 V rf substrate bias impact the wafer with a bimodal energy distribution, as shown in Figure 10(b). For such a thin sheath ($\sim 0.5$ mm), their transit time is $\sim 30$ nsec for the Ar$^+$, which is shorter than the cycle period of the field for 13.56 MHz (74 nsec). This allows the ions to “sense” the instantaneous sheath potential. Since Cl$_2^+$ is almost twice as massive as Ar$^+$, its transit time is longer, $\sim 40$ nsec, and it “senses” the instantaneous potential to a lesser degree while giving Cl$_2^+$ a narrower ion energy distribution width. For both cases, it can also be seen that the Ar$^+$ IEDs are shifted to lower energies than that of Cl$_2^+$, since the rate of energy loss in charge exchange collisions is greater due to the much larger Ar density and the elastic collision energy loss is faster due to more like-mass collision partners.

For the standard biased case, there is nonuniformity in the sheath thickness above the wafer. Near the edge of the wafer, the electron density at the edge of the sheath drops by 20% and the displacement current increases slightly due to the proximity of the thicker, lower capacitance wafer clamp, as shown in Figures 11(a) and (b). Since the thickness of the sheath is proportional to the displacement current and inversely proportional to the electron density, the sheath thickness increases at the outer edge of the
wafer from 0.45 to 0.50 mm, as shown in Figure 11(c). This nonuniformity is noticeable over the 7 to 10 cm radial range of the wafer. This thickening of the sheath increases the transit time of ions by ~5% and leads to a narrowing of the ion energy distributions (see Figure 12), since their transit time will include a larger fraction of the field cycle period. The average ion energy at these outer radii drops slightly, since the sheath voltage also drops due to the capacitive effects of the wafer clamp. The radial nonuniformity is noticeable only over the 8 to 10 cm region of the wafer.

The average incident angle, for ions for the 100 V rf substrate bias, is very uniform across the wafer due to the sheath uniformity, as shown Figure 13(a). An average angle of 8° with an average impact energy of 40 eV corresponds to the ions entering the sheath with ~1 eV, which is reasonable for transit through the presheath region. For the unbiased substrate, the average incident angle is 29°, since the potential drop across the sheath is due only to the dc self-bias giving the ions only an average impact energy of 6 eV. Again, based on the incident angle and the impact energy, the ions enter the sheath with ~1 eV, which agrees with the biased case. As expected, neutrals impact with a 45° angle, as shown in Figure 13(b) due to their almost isotropic velocity distribution.

B. Ion Energy Distributions

In a plasma reactor, the three main parameters that can be changed to adjust the ion energy distributions are the rf bias amplitude on the substrate, the inductive power, and the pressure. The effects of varying these parameters have been studied for the Ar/Cl₂ gas chemistry. The rf bias was varied from 50 V to 150 V, the power was varied from 150 W to 1 kW, and the pressure was varied from 5 mTorr to 20 mTorr.

As the substrate bias is increased, there is the expected increase in average ion energy from 20 eV for the 50 V bias case to 70 eV for the 150 V bias case, as is shown in Figure 14. This corresponds to an average ion energy at the wafer of 5 eV less than the rf bias amplitude, which is due to the actual sheath voltage spending a greater part of the bias cycle at lower voltages, since the sheath is partially resistive. The widths of the distributions for Cl₂⁺ are ~50% of the bias amplitude, since the ion transit time is ~50%
of the bias cycle time. It can also be seen that as the bias is increased, the relative ratio of the low energy peak to the high energy peak decreases. The sheath thickness has increased from 0.25 mm to 0.6 mm and should, therefore, look less capacitive. During the positive fraction of the cycle, the sheath potential drop tracks the sheath voltage with respect to ground, and for increases in bias amplitude the difference between these two changes very little. During the negative fraction of the rf bias, the sheath potential drop increases rapidly as the sheath potential drops away from the sheath voltage with respect to ground. Therefore, as the rf bias is increased, the positive cycle fraction changes little, while the negative cycle fraction contributes to a much larger fraction of the ion flux.

An increase in inductive power for this reactor increases the plasma density almost linearly in this range, which agrees with experiments. This causes a semilinear decrease in the sheath thickness, as shown in Figure 15. There is a corresponding increase in the ion energy distribution widths for both Ar\(^+\) and Cl\(_2\)\(^+\) as the power is increased from 150 W to 1 kW for a 100 V rf bias and 10 mTorr, as shown in Figure 16. Since the Cl\(_2\)\(^+\) is heavier and its transit time is longer than that of the Ar\(^+\), the drop in sheath thickness from 0.88 mm to 0.34 mm has a much greater effect on its IED width. At 0.88 mm, the Cl\(_2\)\(^+\) IED width is only 25 eV, which corresponds to a transit time on the order of 80-85% of the bias cycle time. The Ar\(^+\) IED width is 40 eV, with a sheath transit time of 60-65% of the bias cycle time. At 1 kW, the Cl\(_2\)\(^+\) and Ar\(^+\) IED widths have increased to 57 eV and 65 eV, respectively. The transit times for both species have dropped to only 20-30% of the bias cycle time. Therefore, they are both well into the instantaneous potential regime. The effects of increasing power on Ar\(^+\) and Cl\(_2\)\(^+\) IED widths while varying the substrate rf bias are shown in Figure 17. At low powers, where the sheath is thicker, the Cl\(_2\)\(^+\) IED width is little affected by the increase in bias amplitude, while the lighter Ar\(^+\) shows a much greater effect. At higher powers, where the sheath has thinned, both Ar\(^+\) and Cl\(_2\)\(^+\) show strong changes in their IED widths as the bias amplitude is increased. There is also a drop in average ion energy at the wafer of ~5 eV for an increase in power from 150 W to 1 kW. This agrees with the experiments of Fusakawa et al. and can be attributed to a drop in average sheath potential for the thinner, more capacitive sheath where the conduction to displacement current ratio has increased.
Changes in the gas pressure of the reactor can also strongly affect the IEDs. As shown in Figure 18, increasing the pressure from 5 mTorr to 20 mTorr cause both the IED widths and average ion energy to increase. The increase in IED width and average energy are both due to an increasing dc self-bias, which is produced by the increase in confinement of the plasma for higher pressures. As the plasma becomes more confined, the discharge becomes more asymmetric, since the grounded electrode becomes restricted to the quartz roof and, therefore, much less conductive.

C. Ion and Neutral Fluxes

Ion and Neutral fluxes for an Ar/Cl₂ gas mixture were investigated. The parameters varied were rf bias, inductive power, and pressure, and their affects on the uniformity and magnitude of the fluxes to the surface of the wafer were studied.

Increases in rf bias amplitude at the substrate have very little effect on the magnitude of fluxes to the wafer for either the neutrals, in this case the Cl radical, or the ions, as shown in Figures 19(a) and (c). The ratios of fluxes due to the different ion species show little change as well. There is, however, a slight increase in radial ion flux uniformity, as shown in Figures 19(b) and (d). This is due to greater radial uniformity in plasma density and ion densities in the reactor due to a flattening of the time-averaged sheath potential.

As mentioned before, increases in inductive power lead to near linear increases in plasma density and, therefore, linear increases in all fluxes to the wafer. The Cl radical flux increases linearly from $2.5 \times 10^{17}$ cm$^{-2}$s$^{-1}$ at 150 W to $7.9 \times 10^{17}$ cm$^{-2}$s$^{-1}$ at 1 kW with little change in radial uniformity, as shown in Figure 20(a). The ion fluxes also increase linearly with power with little change in their ratios, as shown in Figure 20(b). There is a slight loss of uniformity for higher powers due to more localized sourcing of the plasma species which occurs at higher conductivities and thinner skin depths.

Finally, increases in pressure can have several effects on the fluxes to the wafer. A linear increase in Cl radical flux due to an increase in its density in the reactor for higher pressures is shown in Figure 21(a). The three ion species fluxes are affected differently by the increase in pressure, as shown in Figure 21. The Cl$_2^+$ flux decreases
slowly and somewhat linearly with increase in pressure, while the Ar$^+$ and Cl$^+$ fluxes decrease much more dramatically and nonlinearly. The Ar$^+$ can charge exchange with both Ar and Cl$_2$, thereby producing some amount of Cl$_2^+$ ions; Cl$^+$ charge exchanges with Cl$_2$, also producing Cl$_2^+$. However, Cl$_2^+$ does not charge exchange with either Ar or Cl. Therefore, there are no nonsymmetric charge exchange channels for the production of Ar$^+$ or Cl$^+$, while there is for Cl$_2^+$. This leads to faster depletion of Ar$^+$ and Cl$^+$ by charge exchange and neutralization reactions with Cl$^-$ than Cl$_2^+$, which has added source channels.

D. Outer Coil Reactor Geometry

The effects of powering only the outer two coils, shown in Figure 22, have been studied for the standard parameters of Ar/Cl$_2$ gas mixture, 500 W inductive power, 10 mTorr, and 100 V rf bias on the substrate. It has been shown that powering only the outer two coils can lead to greater radial uniformity in plasma species densities$^{18}$ due to a drop in sourcing towards the center of the reactor and the effects of diffusion from outer radii removing the local maximum at inner radii. The effects on both the radial uniformity and magnitude of IEDs and fluxes at the wafer were examined.

In Figure 23(a), the peak in density for Cl$_2^+$ has shifted to larger radii for the outer coil, with a somewhat less uniform distribution as well as an 18% drop in maximum density. The effects of this change, as shown in Figure 24(a), are a 40% drop in Cl$_2^+$ flux to the wafer and a slight increase in the relative flux at larger radii. Therefore, uniformity is changed little and the magnitude is decreased.

The Cl radical density in the reactor changes only slightly in spatial uniformity with the loss of the peak region near the center and top of the reactor as seen in Figure 23(b). However, the maximum Cl density has dropped by 45%. These decreases in maximum densities for both the radical and ion are due to less uniform power deposition in the reactor and, therefore, lower overall plasma densities. Figure 24(b) shows a corresponding 45% drop in Cl flux to the wafer and a slight increase in radial uniformity.
For the outer coil geometry, the plasma density is smaller than for the standard case. This leads to an increase in sheath thickness, as shown in Figure 25(a), and a narrowing of the IED width to 30 eV, as opposed to 50 eV for the standard case shown in Figure 25(b). There is also a change in the radial uniformity of the sheath as the peak plasma density is moved to larger radii. There is a slight increase in the sheath thickness for smaller radii due to the relative drop in plasma density there. This leads to a further narrowing of the IED by ~5 eV. The relative increase in high energy peak size in this region is due the thicker, less capacitive sheath.

E. Subwafer Dielectric

A dielectric ring 1.8 cm wide and 1.5 cm thick was placed under the wafer centered at 5 cm to simulate the effects of subwafer topography, such as electrostatic chucks and cooling channels. As shown in Figure 26, this dielectric acts as a relatively small capacitance added in series with the sheath and wafer capacitances. With its smaller capacitance, the dielectric ring can “steal” a large fraction of the potential drop across the sheath. This can lead to large nonuniformities in the IEDs as well as the flux and angular distribution of the ions. This geometry was studied for a pure Ar plasma at 10 mTorr and 100 V rf bias on the substrate at two inductive power levels, 200 W and 800 W.

The dielectric ring has a dramatic effect on the sheath for the high power case, as shown in Figure 27. The average ion energy at the wafer drops from 57 eV to 18 eV over the dielectric, which corresponds to a similar drop in average sheath potential. Also the sheath thickness has changed from greater than 0.10 mm to less than 0.04 mm since the potential is less, which produces a smaller displacement current. The ion energy distribution narrows in this region, however, since a large fraction of the potential is dropped over the dielectric rather than the sheath.

In the low power case, Figure 28 shows that the dielectric has a much less dramatic effect on the sheath uniformity. For lower powers, the sheath is thicker, 0.33 mm, and has a correspondingly smaller capacitance. Therefore, a smaller fraction of the potential is dropped across the dielectric. The sheath thickness changes by only 45%
rather than the 70% change for high power case, and the drop in average ion energy at the wafer is from 60 eV to 37 eV. Therefore, only ~40% of the potential is lost to the ring for the low power case, while 70% is lost for the high power case.

Both high and low power cases show effects of the dielectric ring on the incident angle and flux on ions at the wafer. For the high power case, the average incident angle increases to 12° above the dielectric from 8° over the rest of the wafer, while the low power case shows an increase to only 10° in Figures 29(a) and (c). This is expected due to the drop in vertical acceleration of the ions across the smaller potential over the dielectric ring. The radial flux distributions for both cases, shown in Figures 29(b) and (d), are slightly nonuniform in that there is depression in the flux over the dielectric ring. In this region, the densities of the ions are lowered, since the sheath is thinner than in the areas surrounding.

F. Etching

Using Dane and Mantei’s analytic model\(^3\) for chlorine plasma etching described in Section II.B.v., the etch rates for the Ar/Cl\(_2\) and pure Cl\(_2\) were calculated to examine the effects of rf bias on the substrate, inductive power, and pressure. The radially averaged etch rates were used as well as examination of the radial uniformity of the etch. For the canonical case of Ar/Cl\(_2\) at 500 W, 10 mTorr, and 100 V bias, the radial distribution of the etch rate was determined using the data for the Cl radical flux and the power flux of the ions, as shown in Figures 30(a) and (b). The two factors of maximum neutral etch rate and maximum power flux etch rate were calculated to allow comparison to the actual etch rate and to determine their relative effect. As is shown in Figure 30(c), the maximum power flux etch rate is the larger of the two as well as being less uniform radially. Due to the parallel resistive nature of the etch rate formula, the smaller neutral etch rate dominates. Therefore, the actual etch rate is smaller than either component, and its radial uniformity corresponds more closely to the neutral etch rate. The actual etch rate shows a slight “hump” around 3.5 cm where the power flux etch rate is peaked. In Figure 31, the deviation of the etch rate from the radial mean of 1842 Å/min is portrayed. Except for the outer two centimeters, the deviation remains less than 10%, which is
reasonable for normal etching processes. For a wafer density of $5 \times 10^{22}$ atoms/cm$^3$, this etch rate corresponds to a flux rate of SiCl$_2$ from the surface of $1.5 \times 10^{16}$ molecules/cm$^2$s. For the canonical case, Figure 19(c) shows the average ion flux to the surface to be $\sim 7 \times 10^{16}$ cm$^{-2}$s$^{-1}$. The ratio of ion impacts to etched SiCl$_2$ is, therefore, $\sim 4-5$. This compares well to the results of beam studies$^{22}$ which simulate reactor conditions, as well as Dane and Mantei’s experimental results for their plasma reactor.

By changing the rf bias amplitude at the substrate, the power flux of ions can proportionally be increased and, in principle, the etch rate will increase. However, based on Dane and Mantei’s model, this increase will occur only in the ion power flux limited regime. As can be seen in Figure 32, for low powers and low bias amplitudes, this is indeed the case. When the power is increased and/or the bias amplitude is greater, the system becomes neutral starved, and changes in bias amplitude have little effect. At low power, the ion power flux is near the cutoff of 85 mW/cm$^2$. Increases in bias amplitude contribute to a fast increase in ion power flux limited etch rate from below that of the neutral flux limited etch rate. At higher powers, where the ion power flux is much greater than the cutoff power flux, increases in the bias amplitude contribute to only a linear increase in the ion power flux limited etch rate. The ion component at 50 V bias is almost equal to the neutral flux limited etch rate.

Changes in pressure have a much different effect on the etch rate. Increases in pressure lead to increases in radical flux rates and decreases in ion flux rates to the wafer. As shown in Figure 33(a), at 5 mTorr the power flux limited etch rate is a factor of five larger than the neutral flux limited etch rate, which gives a very neutral starved system. At 20 mTorr, on the other hand, the neutral flux limited etch rate is now the larger by a factor of two, which gives a somewhat ion power flux starved system. The crossover between the two regimes is at approximately 15 mTorr. The actual etch rate in Figure 33(b) shows a strong increase between 5 and 10 mTorr, where the ion power flux drops off dramatically and the neutral flux increases almost linearly. Above 10 mTorr, the ion power flux limited and neutral flux limited etch rates are of comparable size and are decreasing and increasing, respectively, with equal magnitude. In the region, the actual etch rate shows only limited increase due to the slightly faster increase of the neutral flux limited etch rate.
IV. CONCLUSIONS

A Plasma Chemistry Monte Carlo model has been developed to examine the angular and energy distributions as well as fluxes at the wafer surface in high density, low pressure inductively coupled plasma reactors. Input data, such as time-dependent electric fields, plasma species sourcing, and advective flow fields are calculated in a companion 2D hybrid fluid-Monte Carlo model. The model allows for all pertinent reactions in the gas phase as well as reactions on the reactor surfaces including the wafer. The data produced by the PCMCS can be used to examine the properties of the species fluxes at the reactor surfaces and, therefore, the etching of the wafer surface including radial uniformity, anisotropy, and absolute rates.

For the high density, low pressure reactor studied, the sheath thickness had a dramatic effect on the ion energy distributions at the wafer, since ion transit times through the sheath were shorter than the substrate bias frequency (13.56 MHz). For high substrate bias amplitude (150 V) and high ICP power (1 kW) or higher pressures (20 mTorr), this can lead to ions impacting the wafer at energies > 100 eV. For lower powers (150 W) and pressures (5 mTorr), the sheath is thicker and the IEDs are much narrower for the same substrate bias amplitude. Since surface chemistry can be dependent on ion impact energy, narrower ion bombardment energy ranges lead to more predictable etching effects as well as avoiding high energy bombardment damage. Current reactor development has moved towards higher power, higher plasma density reactors due to their etch rates and etch anisotropy. However, these high powers can lead to ion bombardment at energies much higher than expected due to IED widening and, therefore, greater wafer damage, implantation, and nonlinear etching effects.

It was shown that the effects of subwafer geometry can be dramatic, especially at higher powers, due to their effect on the local capacitance and, therefore, the sheath potential as well as its thickness. Ion energy distributions drop in energy and width due to the voltage “robbed” by the added capacitance of the subwafer dielectric materials. Ion fluxes are locally lower due to perturbation of the sheath, and average incident angles of the ions increase due to the drop in the sheath potential. Therefore, at higher powers,
the effects of subwafer topography can strongly affect etch uniformity, and anisotropy and cannot be ignored.

Using Dane and Mantei’s etch model, the uniformity of wafer etching as well as the effects of power, pressure, and bias were presented. The reactor configuration in this study was found to be easily neutral flux starved, except for low bias amplitude and low power or high pressure where the relative ion power flux was low. Therefore, throughout most of the cases, the etch rate and uniformity were controlled mainly by the neutral flux. Increases in substrate bias beyond 50 to 80 V have little effect on etch rate, especially at higher powers; increases in power lead to somewhat linear increases in etch rate, and increases in pressure do not strongly affect the etch rate above 10 to 15 mTorr. These trends follow those found experimentally by Dane and Mantei.
<table>
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<tr>
<th>Gas Mixture</th>
<th>Power (W)</th>
<th>Pressure (mTorr)</th>
<th>Substrate Bias (V)</th>
<th>Other</th>
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### Table 2. Gas phase reactions for 100% Ar.

<table>
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<tr>
<th>Process</th>
<th>Rate Coefficienta</th>
<th>Ref.</th>
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<td>Ar⁺ + Ar → Ar⁺ + Ar</td>
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<td>b</td>
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<tr>
<td>Ar⁺ + Ar → Ar⁺ + Ar</td>
<td>2.217 × 10⁻¹⁰</td>
<td>b</td>
</tr>
<tr>
<td>Ar(hot) + Ar → Ar(hot) + Ar</td>
<td>2.217 × 10⁻¹⁰</td>
<td>b</td>
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<tr>
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<tr>
<td>Ar⁺⁺ + Ar → Ar(hot) + Ar⁺</td>
<td>1.000 × 10⁻⁹</td>
<td>c,24</td>
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</table>

aRate coefficients have units of cm³s⁻¹ unless otherwise noted.
bElastic collision rate coefficients were calculated as described in II.B.iv.
cEstimated.
Table 3. Gas phase reactions for Ar/Cl2 gas mixture.

<table>
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<th>Process</th>
<th>Rate Coefficient$^a$</th>
<th>Ref.</th>
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<tr>
<td>Ar$^+$ + Ar $\rightarrow$ Ar$^+$ + Ar</td>
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<td>Ar$^+$ + Cl$_2$ $\rightarrow$ Ar$^+$ + Cl$_2$</td>
<td>2.348 $\times$ 10$^{-10}$</td>
<td>b</td>
</tr>
<tr>
<td>Cl$_2^+$ + Cl$_2$ $\rightarrow$ Cl$_2^+$ + Cl$_2$</td>
<td>2.356 $\times$ 10$^{-10}$</td>
<td>b</td>
</tr>
<tr>
<td>Cl + Cl$_2$ $\rightarrow$ Cl + Cl$_2$</td>
<td>2.487 $\times$ 10$^{-10}$</td>
<td>b</td>
</tr>
<tr>
<td>Cl$^+$ + Cl$_2$ $\rightarrow$ Cl$^+$ + Cl$_2$</td>
<td>2.487 $\times$ 10$^{-10}$</td>
<td>b</td>
</tr>
<tr>
<td>Cl$^+$ + Cl$_2$ $\rightarrow$ Cl$^+$ + Cl$_2$</td>
<td>2.487 $\times$ 10$^{-10}$</td>
<td>b</td>
</tr>
<tr>
<td>Cl$^+$ + Cl$_2$ $\rightarrow$ Cl$^+$ + Cl$_2$</td>
<td>2.487 $\times$ 10$^{-10}$</td>
<td>b</td>
</tr>
<tr>
<td>Ar$^<em>$ + Ar$^</em>$ $\rightarrow$ Ar$^*$ + Ar + M$^-$</td>
<td>5.000 $\times$ 10$^{-10}$</td>
<td>23</td>
</tr>
<tr>
<td>Cl$^+$ + Cl$^+$ $\rightarrow$ Cl + Cl</td>
<td>1.000 $\times$ 10$^{-7}$</td>
<td>c,25</td>
</tr>
<tr>
<td>Cl$^+$ + Cl$_2^+$ $\rightarrow$ Cl + Cl$_2$</td>
<td>1.000 $\times$ 10$^{-7}$</td>
<td>c,25</td>
</tr>
<tr>
<td>Cl$^+$ + Ar$^+$ $\rightarrow$ Cl + Ar</td>
<td>1.000 $\times$ 10$^{-7}$</td>
<td>c,25</td>
</tr>
<tr>
<td>Ar$^*$ + Cl$_2$ $\rightarrow$ Ar + Cl$_2$ + M$^-$</td>
<td>7.100 $\times$ 10$^{-10}$</td>
<td>28,29</td>
</tr>
<tr>
<td>Ar$^<em>$ + Cl $\rightarrow$ Ar + Cl$^</em>$</td>
<td>7.000 $\times$ 10$^{-12}$</td>
<td>29,30</td>
</tr>
<tr>
<td>Ar$^*$ + Cl$_2$ $\rightarrow$ Ar + Cl$_2^+$</td>
<td>8.400 $\times$ 10$^{-11}$</td>
<td>31</td>
</tr>
<tr>
<td>Ar$^*$ + Cl$_2$ $\rightarrow$ Ar + Cl$^+$ + Cl</td>
<td>6.400 $\times$ 10$^{-11}$</td>
<td>31</td>
</tr>
<tr>
<td>Ar$^<em>$ + Cl $\rightarrow$ Ar + Cl$^</em>$</td>
<td>2.000 $\times$ 10$^{-10}$</td>
<td>c</td>
</tr>
<tr>
<td>Cl + Cl + M $\rightarrow$ Cl$_2$ + M</td>
<td>1.280 $\times$ 10$^{-32}$ cm$^6$/s$^{-1}$</td>
<td>d,26</td>
</tr>
<tr>
<td>Cl$^+$ + Cl$_2$ $\rightarrow$ Cl + Cl$_2^+$</td>
<td>5.400 $\times$ 10$^{-10}$</td>
<td>27</td>
</tr>
<tr>
<td>Ar$^*$ + Ar $\rightarrow$ Ar + Ar$^+$</td>
<td>1.000 $\times$ 10$^{-9}$</td>
<td>c,24</td>
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<tr>
<td>Cl$_2^+$ + Cl$_2$ $\rightarrow$ Cl$_2$ + Cl$_2^+$</td>
<td>1.000 $\times$ 10$^{-9}$</td>
<td>c,24</td>
</tr>
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</table>

$^a$Rate coefficients have units of cm$^3$/s$^{-1}$ unless otherwise noted.

$^b$Elastic collision rate coefficients were calculated as described in II.B.iv.

$^c$Estimated.

$^d$Three body rate coefficient with M being any other gas species.
REFERENCES


26 NIST Chemical Kinetics Database Version 5.0, (National Institute of Standards and Technology, Gaithersburg, MD, 1993).


Figure 1. Flowchart of 2D hybrid model for inductively coupled plasma reactors.
Figure 2. Vector representation of advective flow velocities for (a) full reactor and (b) closeup of region near inlet.
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