Influence of modeling and simulation on the maturation of plasma technology: Feature evolution and reactor design

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Plasma materials processing for microelectronics fabrication, formerly an empirical technology, has in recent years greatly benefited from the use of modeling and simulation (MS) for equipment and process design. The maturation of plasma equipment and feature scale MS has resulted from a better understanding of the underlying physics and chemistry, from innovation in numerical algorithms and in the development of a more comprehensive fundamental database. A summary is presented of the historical development, present status and future potential of MS for feature evolution and plasma reactor design. © *2003 American Vacuum Society.* [DOI: 10.1116/1.1600447]

I. INTRODUCTION

Modeling and simulation (MS) of equipment and processes for plasma modification of materials for microelectronics fabrication is best described by a hierarchy of goals: testing fundamental understanding, assisting in the development and interpretation of experiments, and performing *a priori* design of new processes and apparatus. MS has met and exceeded the first two of these goals. The future legacy for MS is the degree to which the third goal will be met. MS in plasma processing encompasses two conceptually different but tightly linked activities: modeling of gas phase reactor scale dynamics and simulation of surface feature scale processes. The reaction chemistry of surfaces provide boundary conditions for reactor scale processes; and simulation at the feature scale requires fluxes from reactor scale phenomena. To achieve the goal of using MS for first principles design of equipment and processes, these two scale lengths must ultimately be linked in a self-consistent fashion.

The complexity and difficulty of MS for plasma processing is largely a consequence of the systems of interest being in a parameter space where conventional approximation techniques are either poor or invalid; and so first principles approaches are either preferred or necessary. MS in plasma processing stands out for having developed innovative computational techniques and for leveraging computational techniques developed for other fields. In spite of these complexities, MS has made impressive progress toward both improving our fundamental understanding of and providing design assist for new equipment and processes. MS also holds high promise for revolutionizing innovation of new materials and structures. MS has made contributions to the design of plasma tools both in development and on the production line. In this article, overviews of progress and future challenges for feature scale and equipment scale modeling will be presented.

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II. FEATURE SCALE PROFILE EVOLUTION

Obtaining the desired feature shape in a microelectronic device, uniformly across the wafer, is the goal of the plasma processing engineer. Today this optimization is largely an empirical exercise. Models employing empirically adjusted parameters provide insights that suggest strategies to use for optimization or process correction. Example of profile evolution simulation packages include SPEEDIE, EVOLVE, and SIMBAD.[1–3]

At each point along a surface defining a feature, species impact and leave the surface, as shown in Fig. 1. Positive ions impact and may reflect and, in some cases, electrons and possibly negative ions may also enter the feature. Neutral species are incident from the plasma or are reflected, desorbed or generated within the feature, impacting at all surface sites. Species and charge can also be transported along surfaces or into and out of the subsurface region. Adjacent features may also play a role in defining the shape of a feature because of shadowing or through more complex physiochemical interactions. Surface composition, roughness, stress and voltage, among other variables, will influence the transport and reactivity within the feature.[4]

The first task for feature evolution MS is predicting how the interface defining the solid surface is advanced in time and space. The surface advance problem can be thought of as the solution $\mathbf{F}$ to the partial differential equation: $\partial\mathbf{F}/\partial t + \mathbf{R}\cdot\nabla\mathbf{F} = 0$, in which the surface is defined by the value of function $\mathbf{F}(\mathbf{r},t) = 0$.[4] The surface shape evolution requires knowledge of the velocity of the interface, $\mathbf{R}$, and a method to discretize the surface. The interface evolution problem has been addressed in many different contexts from fluid dynamics, crystallization, combustion, geophysical, and astrophysical processes. String or cell methods have been used to discretize the surface while a variety of methods have been used to predict the frontal advance.[5] Although there are still challenges remaining in the numerical solution of the interface evolution equations, especially in three dimensions, its status is probably the most mature part of the problem.[5,6]

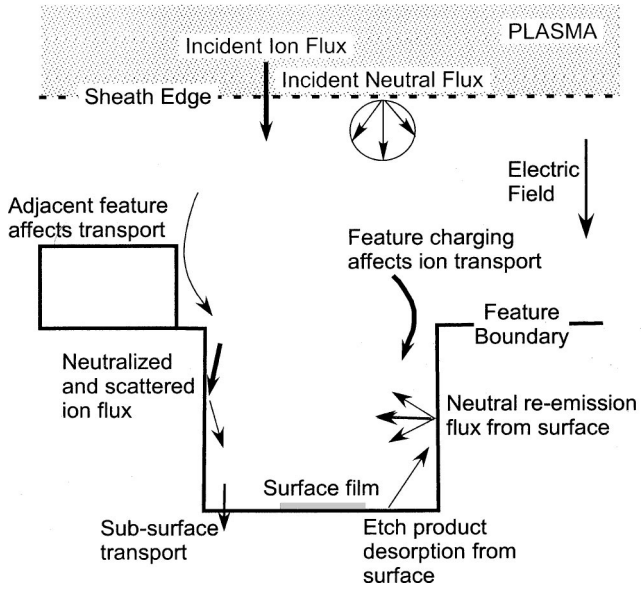

FIG. 1. Schematic of species impacting a microfeature at the wafer surface during plasma processing. Ions and neutral species from the plasma impact, react, reflect, desorb, and are transported into the subsurface region.

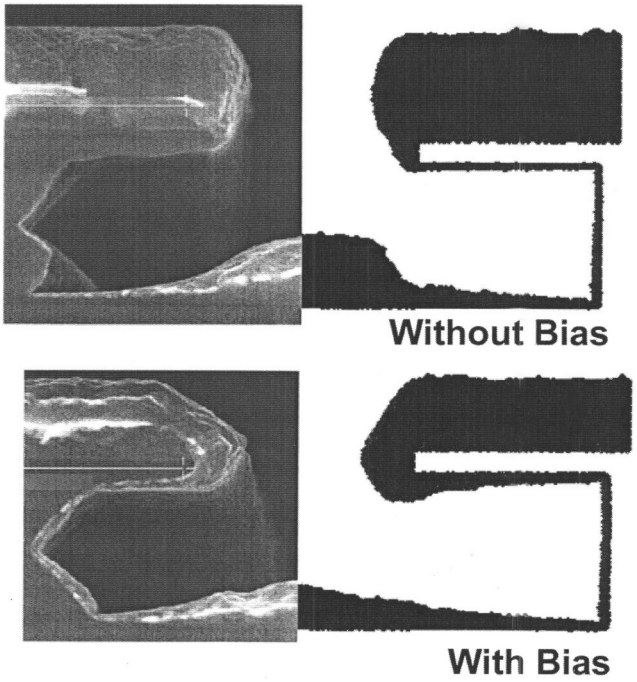

FIG. 2. Test structures are used to deconvolute the relative roles of ion-enhanced and neutral mechanisms. External or line of sight surfaces are exposed to both ion-enhanced and neutral components but interior surfaces not within a direct line-of-sight of ions experience only neutral reactions or reactions of reflected neturalized ions. (Top) Test structure (experiment on left, model on right) for ionized metal physical vapor deposition (IMVPD) without a substrate bias; (Bottom) with a substrate bias (adapted from Ref. 8).

Transport within a feature is typically collisionless. Integral expressions summing the contributions of species arriving at all angles within the line of sight of any given point on the surface of the feature are often used to model intrafeature transport.[6,7] Trajectories of charged species entering the feature are modified by intrafeature electric fields which, for insulating surfaces, may evolve as the local surface charge density changes. Even if the impacting charged species is neutralized, the reflected neutral species may retain considerable energy. Monte Carlo methods are popular for solution of the governing integro-differential equations describing transport of charged and neutral species within the feature.

A reaction between an impacting species and the surface can lead to either deposition or etching. The contributions to **R** at surface reactive sites are balanced between adsorption and desorption of either deposition or etching precursors. The ratios of ion to neutral fluxes, as well as ion energies and angle of impact, are used to develop semiempirical surface rate expressions. Parameters such as reactive sticking coefficients at open sites, stoichiometric coefficients for etch products, ion-assisted chemical or physical sputtering yields, and parameters for all of the composition-dependent, energy-dependent, and angle-dependent expressions are adjusted to match model prediction of feature shape to experimental data in the form of scanning electron micrographs.

One effective scheme to extract parameter values from measured profiles involves the use of test structures, as shown in Fig. 2.[7,8] Positive ions and highly reactive neutrals tend to react just below the opening. Neutrals that deposit but with a lower reactive probability will tend to adsorb and desorb many times within the cavity, resulting in a more conformal internal distribution. By using a profile simulator with adjustable parameters and comparing to experiments, it is possible under some conditions to assign physically meaningful values to parameters.

A more common approach is to match model predictions with measured feature profiles with conventional lithographic structures. The challenge is to assemble enough information for a range of plasma conditions to infer parameter values. Another strategy is to utilize systems in which the species impacting the surface have been characterized, for example in a vacuum beam system.[9–11]

Profile simulations have been central to efforts to associate the physico-chemical mechanisms with feature shape evolution anomalies such as microtrenching and notching.[10,12–14] One mechanism proposed for microtrenching is near-specular reflection of ions from sidewalls. Molecular dynamics simulations support the hypothesis that ion scattering from feature sidewalls is generally responsible for microtrenching, although the distribution of ion scattering angles was shown to be quite sensitive to surface roughness at the atomic scale, an effect rarely included in profile simulators.[15–17] (See Fig. 3.) Some combination of surface charging resulting in deflection of ion trajectories and stress-induced spontaneous etching are thought to be responsible for notching.[10–14] Experiments have tried to exploit notching in gate electrode etch to reduce the effective device gate length with resolution well below current limits of optical lithography.[18] On the other hand, the use of plasmas to trim photoresist to reduce the feature critical dimensions in gate

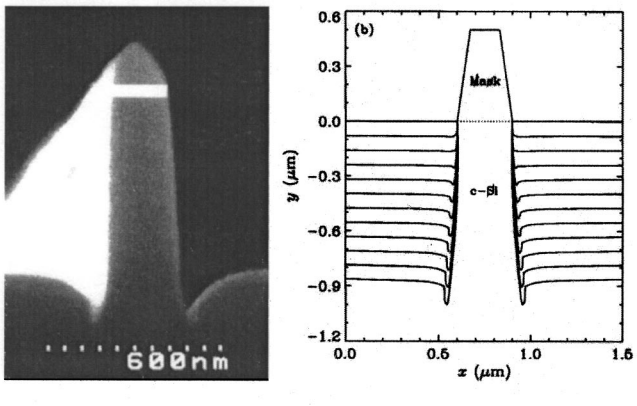

FIG. 3. Consequences of ion scattering on microtrenching of Si in a Cl_2 inductively coupled plasma. (Left) experiment, (right) model (adapted from Ref. 17).

electrode etch below lithographic limits has been widely applied in industry, and profile simulation has played a key role in the development of this technique.[19]

III. EQUIPMENT SCALE MODELING

The fundamental knowledge bases for plasma equipment modeling trace their roots to investigations of microwave breakdown, lamps and lasers during 1960s, 1970s, and early 1980s. The characterization of electron swarms resulting in non-Maxwellian electron energy distributions (EEDs), first investigated in the context of microwave breakdown, produced a computational infrastructure for solving Boltzmann's equation and for modeling complex gas chemistries.[20] Innovative approximation techniques for EEDs (e.g., two-temperature distributions) provided much needed intellectual bridges until improved computing resources enabled more rigorous treatments.[21]

The development of high power lasers in the 1970s and 1980s motivated innovations in MS to aid in their scaling. The first global, one-dimensional and two-dimensional plasma chemistry models, computational techniques later used in plasma processing, trace their origins to these investigations.[22–24] These works were fundamentally less difficult than today's MS for materials processing due to a fortuitous set of operating parameters. Most of these systems operated at pressures and frequencies for which approximate solutions (such as local-field approximations) were quite accurate. Surface reactions, other than charged particle recombination and simple reassociation of radicals were largely ignored, in part because they were not important to the outcome and partly out of the modeler's inexperience. Similar progress was made in use of MS for lamps and arcs using high pressure local-thermodynamic equilibrium (LTE) and low pressure nonequilibrium sources (such as fluorescent lamps). Multidimensional fluid codes were developed for LTE lamps beginning in the early 1980s with progressively pressure increasing levels of sophistication into the 1990s.[25]

The success of MS for lamps, lasers and atmospheric pressure plasma chemistry was in large part a consequence of unprecedented devotion of resources to the development of the fundamental knowledge bases in atomic and molecular physics, and in computational techniques. Today's availability of electron impact cross sections, ion mobilities, analysis techniques and data for ion–molecule reactions can in large part be traced to these efforts.[26,27]

The use of radio frequency (rf) technologies for plasma processing was, to some degree, an unprecedented challenge to the plasma modeling community. These operating conditions were precisely in that range where virtually all previous approximations were no longer valid. Mean free paths were not small fractions of reactor dimensions but suddenly large fractions. Equilibration times were suddenly neither very long nor very short compared to the harmonic period. Chemically reactive surfaces were suddenly critical to the state of the plasma, not inconsequential.

The first progress towards equipment scale modeling for plasma processing occurred in global modeling in the early 1980s using techniques patterned after their predecessors for lasers to produce volume averaged densities of electrons, ions, and radicals.[28,29] With simplifying assumptions predictions of etching and deposition rates were made. Global modeling of greater sophistication now provides a rapid and intuitive method to investigate plasma chemistry and nonlinear phenomena.[30,31]

The realization that the dynamics of the sheath are critical to the operation of rf discharges resulted in specialized modeling activities which provided much needed insight to these complex structures and which were later incorporated into equipment models.[32,33] Monte Carlo and particle-in-cell methods were also used to investigate the consequences of sheath dynamics on electron transport.[34,35] Monte Carlo and semianalytic methods were used to investigate the acceleration of ions through sheaths and their resulting distribution of ion energies and angles onto the substrate.[36,37]

Beginning in the early to mid 1980s the first spatially dependent models for the plasma chemistry of capacitively coupled etching and deposition systems began appearing. These were rapidly followed by models which more accurately addressed electron and ion dynamics coupled to Poisson's equation for the electric potential. Many innovative techniques were developed to investigate these dynamics, including continuum, beam-bulk, Greens function, particle-in-cell, and Monte Carlo-fluid hybrid.[38–41] As our fundamental understanding of these systems improved, and computational resources increased, multidimensional models appeared in the late 1980s to early 1990s.[42]

When electron cyclotron resonance and inductively coupled plasmas (ICPs) came to the forefront in the early-to-mid 1990s, MS was well poised to make important contributions to improving our fundamental understanding of these devices and in design of equipment. Simulations for ICPs were generally two dimensional from their first introduction and, soon thereafter, three dimensional.[43–46] (See Fig. 4.) Investigations quantified mechanisms of power deposition, charged particle and neutral transport and how to control uniformity. The use of equipment scale MS for design and

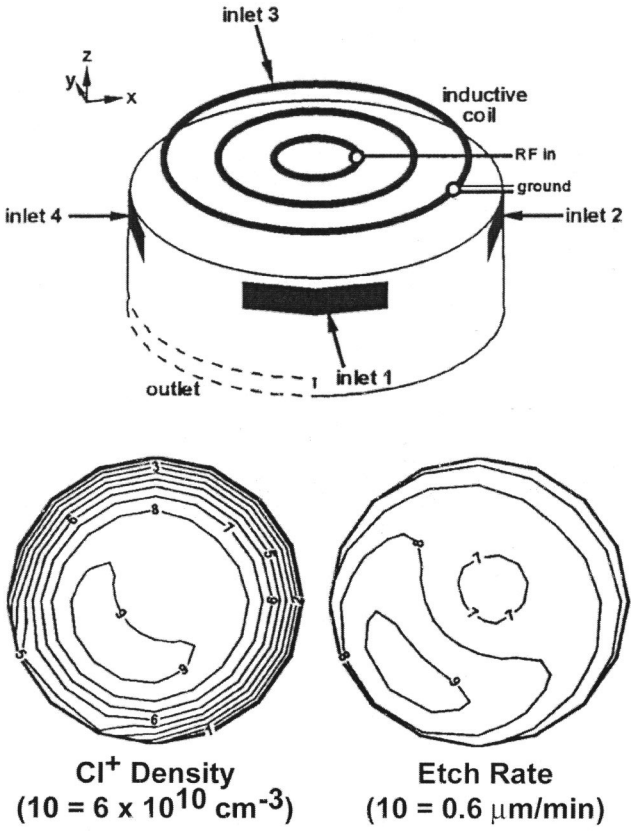

FIG. 4. Asymmetric gas pumping in an inductively coupled plasma can produce asymmetries in ion densities and etch rates, as demonstrated by results from a three-dimensional plasma equipment model for an ICP sustained in 10 mTorr, Cl_2 (adapted from Ref. 45).

optimization of new plasma tools was first truly successful for ICP systems. These reactor scale models also provided platforms for investigating fundamental issues in plasma physics and plasma chemistry, such as nonlocal electron transport and electromagnetic wave–plasma interactions.[47]

In the late 1990s and early 2000s, models integrated more physical phenomena in a self-consistent fashion. More sophisticated models for electric circuitry, electron, and ion transport and surface chemistry, as well as more sophisticated numerical techniques, have enabled investigation of a variety of phenomena, such as multifrequency excited and pulsed plasmas.[48,49] (See Fig. 5.) Reactor scale models were also integrated with feature scale simulations to access reactor parameters on critical dimension control of features.[50]

IV. FUTURE DEVELOPMENTS

Current projections of field effect transistor scaling suggest that sub-10 nm gate length devices will appear in production sometime after 2010.[51,52] Given the extraordinary power to manipulate and control surfaces with plasmas, plasma technology will likely to continue to be at the heart of the manufacture of these devices. New challenges include the introduction of new materials, atomic scale dimensional control, patterning challenges, and damage and contamination control. The challenges for MS in describing feature

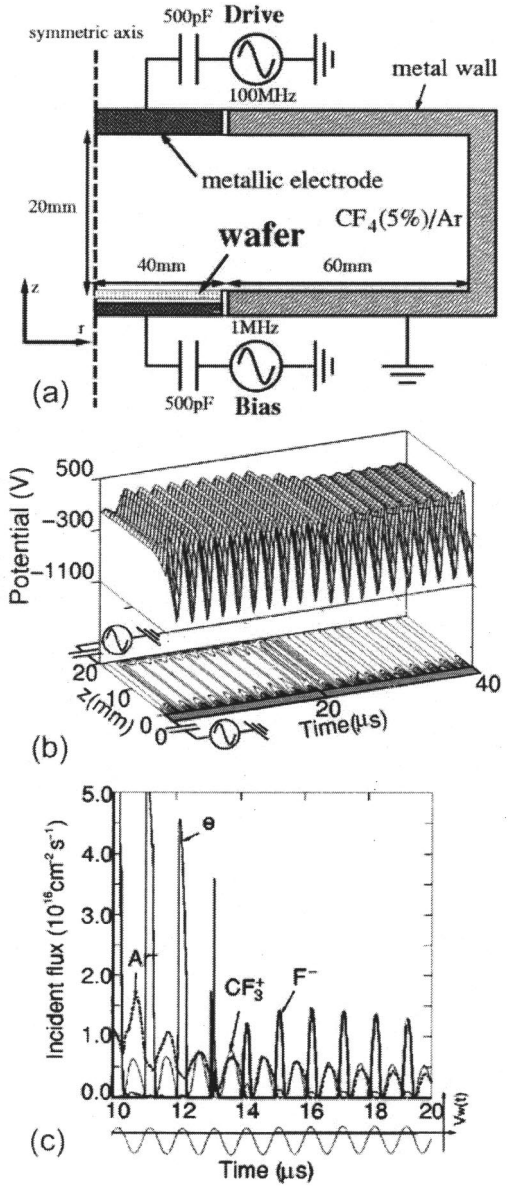

FIG. 5. Modeling results for a pulsed dual frequency capacitively coupled discharge sustained in Ar/CF_4: (a) geometry, (b) plasma potential on the centerline as a function of time, and (c) flux of radicals to the substrate during the time when only the low frequency power is applied (adapted from Ref. 49).

scale properties will also continue to evolve since future devices will likely be hybrids with conventional silicon-like device structure and function coupled with molecular components. Molecular dynamics and Monte Carlo methods, especially designed to handle the range of relevant length and time scales, will be needed to model the molecular-scale surface structures. To meet these challenges, reactor scale MS will also need to address larger dynamic ranges in space and time by the more robust coupling of electromagnetic and plasma transport phenomena while accessing more completely populated databases. Technology solutions may come from innovations in atmospheric-pressure and microplasma

devices and so new algorithms and models should have the necessary robustness and dynamic range to address these possibilities. The self-consistent integration of reactor scale and feature scale models will ultimately provide insight and design capability to optimize these advanced microelectronics devices.

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