DIAGNOSTICS AND MODELING OF PLASMA PROCESSES

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INTRODUCTION

The full exploitation of rf and dc glow discharges for microelectronic and photonic device fabrication, coherent and incoherent light sources, and high voltage switching will only be realized when we have reliable numerical models with which processes can be simulated. It is perhaps ironic that we can simulate device operation[1] in great detail but must resort to trial and error development for device fabrication. This dichotomy is more remarkable when one realizes that the physics of semiconductor devices and plasma reactors are identical. Chemistry complicates the modeling of plasma reactors.

This talk will focus on recent fluid models of discharge physics and *in situ*, non-intrusive diagnostic experiments designed to test these models.[2–8] Specific examples related to diamond film growth and hydrogen-containing plasmas will be highlighted as appropriate. Emphasis will be placed on experimental and theoretical results for electric fields, ion densities, reactive atomic concentrations, and degrees of dissociation.

ELECTRIC FIELDS

Consider sheath electric fields. Understanding the magnitudes and shapes of sheath fields constitutes the most basic understanding of a discharge. The local sheath field depends on not only the applied field but also the space charge distribution. In one dimension, Poisson's equation is solved to obtain the local field:

$$\frac{\partial E}{\partial x} = \frac{e}{\varepsilon_0}(n_p - n_e - n_n) \qquad (1)$$

where n_p, n_e, and n_n are the positive ion, electron, and negative ion densities, respectively, and E is the electric field. Electric fields can be measured non-intrusively and with high spatial and temporal resolution by exploiting molecular and/or atomic Stark effects.[6,9–12] Positive ion densities in Eq. 1 can be measured by laser-induced fluorescence spectroscopy.[13–15] Negative ions can be probed using photodetachment spectroscopy.[7,8,16] Combined, this set of measurements provides stringent tests for theory.

LOCAL FIELD AND BEAM ELECTRON MODELS

The simplest fluid theories entail the solution of Poisson's equation above coupled with equations of continuity for ion and electron densities:

$$\frac{\partial n_i}{\partial t} + \frac{\partial (n_i u_i)}{\partial x} = F - L \qquad (2)$$

where i denotes p, e, or n, u is the average (fluid) velocity, F is the rate of formation, L is the rate of loss. When the local field approximation is valid, *i.e.* the collisional mean free paths are much smaller than the distances over which electric fields and densities change significantly, the source and loss terms in Eq. (2) can be expressed as functions of just E/N. Following this approach, Boeuf[2] recently calculated sheath fields and charge densities in rf discharges through He and obtained good *qualitative* agreement with measurements of sheath electric fields in both low and high frequency discharges containing BCl_3.[6]

Although the local field approximation works reasonably well for electric fields and current-voltage characteristics, it fails miserably for the calculation of ionization and excitation rates. In the sheaths, the electric field varies so rapidly in both space (and time for rf discharges) that the electron energy distribution and electron-impact collision rates are not unique functions of the local value of E/N. To deal with this problem, Graves *et al.* and Sawin *et al.* have expressed the ionization rate coefficient as a function of the average electron energy, which is determined by solving the electron energy conservation equation simultaneously with the continuity and Poisson equations.[3–5] In this fashion, excellent agreement was obtained between calculated and measured space-time dependent optical emission intensities in high frequency discharge.[5,17]

An alternative approach to using an electron energy balance equation is to use electron beam models.[18–20] Electrons created by secondary emission processes at the cathode are considered as a separate group from bulk electrons. Continuity and energy balance equations for these ballistic or beam electrons are solved along with Poisson's equation and continuity equations for bulk electrons and ions. Results from such beam models show good agreement with experiment.[20]

MULTI-DIMENSIONAL EFFECTS

Up until now, the modeling of dc and rf discharges has been mostly limited to one-dimensional systems. Although most parallel-plate reactors can be operated in quasi-one-dimensional regimes and careful experimental design can ensure one-dimensional measurements, most plasma processes do not utilize well-confined discharges. Thus, multi-dimensional effects are important. Recent work at low frequency shows that the electron-beam model is a useful framework within which the ion transport and electric field profiles of asymmetrical parallel-plate discharges can be understood.[21] For example, radial ion density profiles are non-uniform in asymmetrical discharges because the electron beam responsible for ionization has smaller cross sectional area when the small electrode is the momentary cathode than when the large electrode is the momentary cathode. Because the electron beam is created mostly by ion-impact collisions with the electrodes, the non-uniformity is reinforced on every half-cycle. These effects lead directly to non-uniform thin film etching and deposition rates. Although beam models qualitatively explain a variety of ion density and electric field measurements in these asymmetrical discharges, it remains to model these data self-consistently and quantitatively.

REACTIVE SPECIES

Another area for model improvement involves the prediction of reactive species densities.

Although there are numerous models for predicting these quantities, they generally lack self-consistency. The models have either been semi-empirical or have made assumptions about the electric field profile. The simplest chemical discharges to model are those through diatomic gases such as N_2 or H_2. Using 2 photon laser-induced fluorescence, the concentrations of reactive atoms such as N and H can be measured and compared to the results of fluid simulations.[15,22–24] Using spontaneous Raman spectroscopy, it should be possible to calibrate these measurements and also determine the degree of dissociation.[25]

SUMMARY

The use of reliable discharge models for predicting sheath electric field profiles, ion and electron currents, reactive species concentrations, and degrees of dissociation will alleviate the tortuous nature of trial-and-error process development. The optimal process parameter space can be derived more rapidly, key parameters for improved process control can be more readily identified, and data from process monitors can be more easily interpreted and exploited in a feedback control system.

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