Cambridge University Press
978-1-107-41028-2 - Materials Research Society Symposium Proceedings: Volume 165: Characterization of Plasma-Enhanced CVD Processes
Editors: Gerald Lucovsky, Dale E. Ibbotson and Dennis W. Hess
Excerpt
More information

PART I

Diagnostics and Modelling

Cambridge University Press
978-1-107-41028-2 - Materials Research Society Symposium Proceedings: Volume 165: Characterization of Plasma-Enhanced CVD Processes
Editors: Gerald Lucovsky, Dale E. Ibbotson and Dennis W. Hess
Excerpt
More information

PECVD RF DISCHARGE MODELS REVIEW

ALAN GARSCADDEN

Wright Research and Development Center
Wright-Patterson AFB, Ohio, 45433

ABSTRACT

This paper presents a concise and subjective summary of the rapid progress that has been made in the understanding of the essential features of RF discharges. The paper concentrates on introducing the important concepts used in modeling the rf discharge. The discharges have been modeled from several distinctly different approaches. These include circuit, beam-diffusion, plasma fluid or continuum, and particle kinetic models. The treatments have their usefulness depending on the application. The circuit models give easily parameterized results, power deposition, and phase angles between voltage and current, however, they do not describe the important plasma chemistry and the source terms for deposition and etching. The newer continuum models efficiently give self-consistent plasma parameters for higher pressure discharges but synergistic ion and neutral interactions with surfaces are difficult to include. The particle kinetic models can include many effects without approximations, however they need extensive data sets and long computer run times. The coupling of improved diagnostics and the different theories has resulted in a convergence of their conclusions. There are four distinct energy-gain mechanisms in the RF discharge : a bulk plasma excitation; electron beam excitation resulting from secondary emission from ion collisions with the electrodes; wave-riding acceleration on the sheath oscillation (collisional: Kushner); and a non-collisional plasma electron-sheath boundary interaction (Godyak). The relative contributions are sensitive functions of the gas mixture, pressure, frequency and RF voltage.

INTRODUCTION : BASIC INTERACTIONS IN THE RF DISCHARGE

Ionization and excitation in radio-frequency (rf) discharges have several important characteristics that are markedly different from those of direct current (dc) discharges. First, since the applied electric field reverses periodically, at sufficiently high frequencies the charges will not all be swept out of the volume to the electrodes or insulating walls, and the losses are significantly reduced. Thus the breakdown voltage and the operating voltage of the rf discharge can be quite low compared to the dc discharge values. Secondly, under these rf discharge conditions, secondary emission processes at the electrodes are not necessary conditions for the maintenance of the discharge. Plasmas therefore can be excited with external electrodes. Thirdly, if the electrodes are capacitively coupled to the rf generator, the electrodes acquire a negative self-bias due to the requirement that the net charge collected over a cycle must be zero. If the applied voltage is increased, most of the increase occurs across the sheaths and other energy deposition mechanisms become more important. The discharge divides into two quite different regimes : the bulk plasma which resembles the positive column of the dc glow discharge, and the electrode sheath regions.

Studies of the rf discharge have led to the identification of the four principal energy deposition mechanisms identified in Table 1. These are (i) the impedance of the bulk plasma (ii) the energy deposition by fast electrons created by secondary emission due to ion bombardment of the electrodes (iii) collisionless absorption due to the asymmetrical sheath boundary-plasma electron interaction and (iv) wave-riding, or collisional sheath interactions causing electron heating in the sheath modulated electric field. Under these conditions the electron is regarded as surfing on the expanding sheath field. Processes (iii) and (iv) are related with the difference being that in (iii) electron collisions occur during the sheath expansion. There is often an additional interaction due to the changes in the complex impedance (capacitive sheaths and resistive bulk plasma) of the discharge and the consequent changes in the power transferred from the rf generator. Other less general plasma modes occur often due to resonance when the electric field and period are such that one electron transit requires one half period of the rf cycle. Under these conditions at very low pressures when the electron mean free path is larger than the gap spacing and secondary electron emission due to electrons can occur, one has the multipactor discharge mode; when the mean free path corresponds approximately to small integral fractions of the gap spacing then plasmoid modes are excited.

THEORETICAL APPROACHES TO DESCRIBE THE RF DISCHARGE

Modeling of the rf discharge has taken many different approaches, with rapid developments taking place in recent years. These approaches have included:

(i) circuit models, treating the electrode sheaths as leaky variable capacitors and the bulk plasma as mainly resistive.

(ii) beam-diffusion models, treating the electron energy distribution function (EEDF) as bimodal and time-dependent.

(iii) bulk plasma models that neglect the sheaths and assume local equilibrium with the instantaneous local applied electric field (In spite of these severe assumptions reasonable agreement has been obtained in some electronegative gas discharges).

(iv) continuum, or hydrodynamic models that seek a self-consistent spatial and temporal profiles of the electric field. Either local equilibrium (discussed below) or a prescribed EEDF is assumed.

TABLE 1

RF DISCHARGE ENERGY DEPOSITION

REGIMES	CHARACTERISTICS	COMMENTS
POSITIVE COLUMN	TIME - VARYING UNIFORM FIELD	HIGHER PRESSURES ELECTRONEGATIVE
SECONDARY EMISSION	ENERGY MODULATED BEAM	LOW PRESSURES LOW FREQUENCY
WAVE - RIDING	COLLISIONAL LOSSES NEAR SHEATH EDGE	LOCALIZED ENERGY BALANCE
SHEATH REFLECTION	TRANSIT TIME DEPENDENT STOCHASTIC EFFECTS	LOW PRESSURES RARE GASES MULTIPACTOR EFFECTS POSSIBLE

TABLE 2

SELF-CONSISTENT CATHODE SHEATH MODELS

FLUID EQUATIONS	BOEUF BAYLE ET AL SAWIN ET AL
COLLISIONLESS SHEATH	LANGMUIR GODYAK KELLER, PENNEBAKER
COLLISIONAL SHEATH	LIEBERMAN
MONTE-CARLO	BOEUF & MARODE AN & MARODE DOUGHTY OHUCHI & KUBOTA
PARTICLE SIMULATION	SURENDRA & GRAVES
CONVECTIVE-SCHEME	SOMMERER ET AL
METHOD OF CHARACTERISTICS AND BOLTZMANN EQUATION	LONG
BOLTZMANN EQN & EXPANSION METHODS	PITCHFORD TAGASHIRA ET AL

(v) particle models that may derive the electric fields of the sheaths and the bulk plasma self-consistently . These models use various techniques, often derived from high-energy plasma studies and include particle-in-cell (PIC) and Monte-Carlo (MC) approaches.

Godyak [1] has summarized the studies leading to his identification of collisionless heating at the sheath-plasma boundary. When the rf frequency is much less than the electron plasma frequency, the plasma acts like a reflector. Godyak credits Landau [2] with the recognition that there will be an rf field dissipation associated with this shielding. More recent studies by Lieberman [3] emphasize the stochastic nature of the process and also link the collisionless and collisional sheath regimes. The experimental data for argon of Bletzinger [4], in figure 1, illustrate some of the main and unusual features of the rf discharge. The discharge impedance reached a minimum for all frequencies (7 to 20 MHz) at a pressure of about 1 Torr and the impedance decreased with increasing frequency. Below 1 Torr the impedance was independent of the electrode spacing. Adding an attaching gas caused the impedance to increase and the impedance minimum to be at lower pressures. The fact that at the lower pressures the resistive part of the impedance is independent of pressure and spacing indicates that volume collisional losses no longer dominate the discharge.

Analytical studies by Townsend and Gill [5] using a characteristic electron approach led to the definition of the bulk plasma impedance and of the effective rf field. An electron in vacuum in an alternating electric field oscillates 90° out of phase with the field and cannot, on average, receive energy from the field. The electron gains energy from the rf field only if it encounters phase changing collisions. The electron equation of motion in the presence of collisions of frequency ν is:

$$m\,\dot{\bar{u}} = -e\bar{E} - m\nu\bar{u} \qquad (1)$$

For time variations of the quantities as exp(iωt), the electron velocity is:

$$\bar{u} = \frac{e\bar{E}}{m(\nu + i\omega)} \qquad (2)$$

and the electron current:

$$\bar{j} = ne\bar{u} = \frac{ne^2\bar{E}}{m}\frac{(\nu - i\omega)}{(\nu^2 + \omega^2)} \qquad (3)$$

The power into the plasma is then:

$$\frac{ne^2E^2}{2m}\frac{\nu_m}{(\nu_m^2 + \omega^2)} \qquad (4)$$

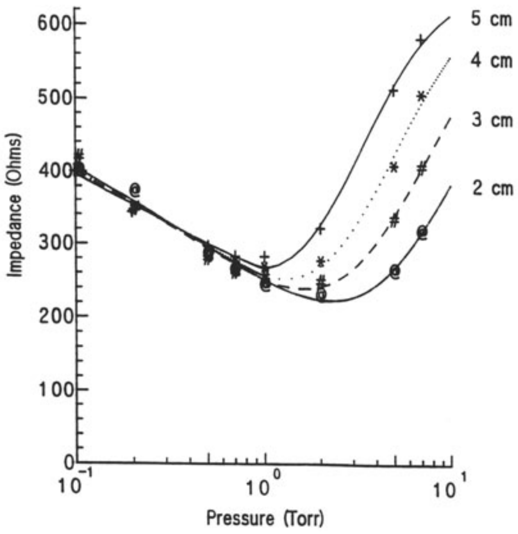

FIGURE 1 RF discharge Impedance at 14.1 MHz in argon as function of pressure and interelectrode spacing (after P. Bletzinger, 1989).

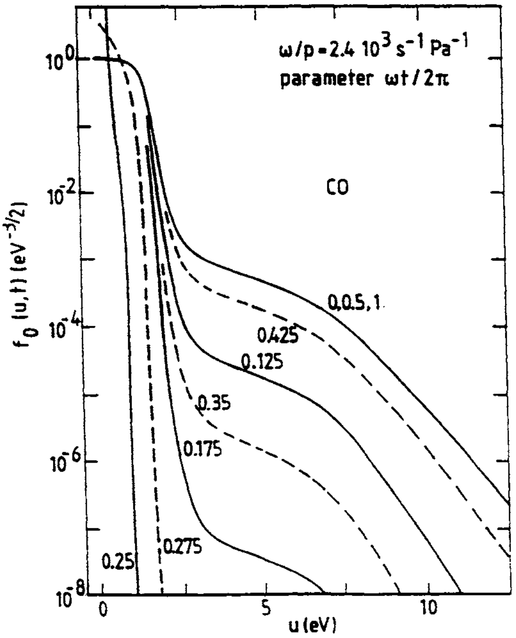

FIGURE 2 The modulation of the isotropic part of the EEDF at low excitation frequency in carbon monoxide. Parameter is normalized phase ample (after Winkler et al, 1986).

Comparing this expression to the power into a dc discharge:

$$\frac{ne^2E^2}{m\nu_m} \tag{5}$$

led to the definition of the effective field as:

$$E_{eff}^2 = E^2\frac{\nu_m^2}{(\nu_m^2 + \omega^2)} \tag{6}$$

This concept was used, in conjunction with solutions of the Boltzmann Transport Equation (BTE) by Margenau [6], and Brown and co-workers [7] to analyze the high frequency discharge in various rare gases.
Note that in spatially non-uniform rf electric fields the charges experience asymmetrical forces and they are driven to regions of lower field. The direction of this force is independent of the sign of the charge. This driving force is:

$$\overline{F} = \frac{e^2}{4m\omega^2}\frac{d(E^2)}{dx} \propto \frac{d(\text{field energy density})}{dx} \tag{7}$$

Extending the characteristic particle approach, Harries and von Engel [8] showed that at low frequencies, $\omega < \nu_r$, (ν_r= energy relaxation frequency), the average electron energy was almost 100% modulated, whereas at higher frequencies, $\omega > \nu_r$, the electron energy showed much smaller modulation around a higher time-averaged value. This same phenomenon shows up very clearly in time-dependent Boltzmann calculations of Winkler et al [9]. As illustrated in figure 2, at low frequencies the whole EEDF is modulated, while figure 3 shows that at high frequencies the EEDF is quasi-stationary, showing modulation only in high inelastic collision frequency energy intervals. For gases like CO and N_2, this causes the modulation to persist at higher rf frequencies over the energy ranges for vibrational excitation and above the thresholds for electronic excitation and ionization. Therefore the effective field approach can be used to a good approximation at microwave frequencies in the rare gases, however it may not applicable at typical rf frequencies in molecular gases with large energy loss frequencies (i.e. cross sections). To obtain accurate radical and ion production rates for the bulk plasma in low frequency rf discharges, it is necessary to average the time-dependent excitation function over the cycle.

LOCAL FIELD EQUILIBRIUM

In the above analyses, one is applying the approximation of local field equilibrium in the Boltzmann transport equation analyses. By this statement we mean that the EEDF can be characterized uniquely by the local value of E/N, where E is the electric field and N is the gas number density. Note that the

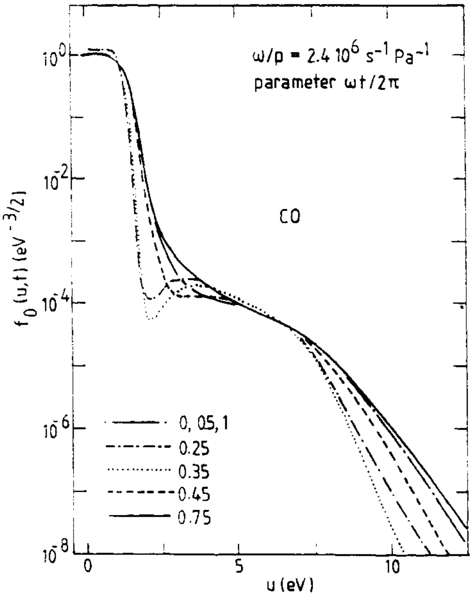

FIGURE 3 The modulation of the isotropic part of the EEDF at high excitation frequency in carbon monoxide (after Winkler et al, 1986).

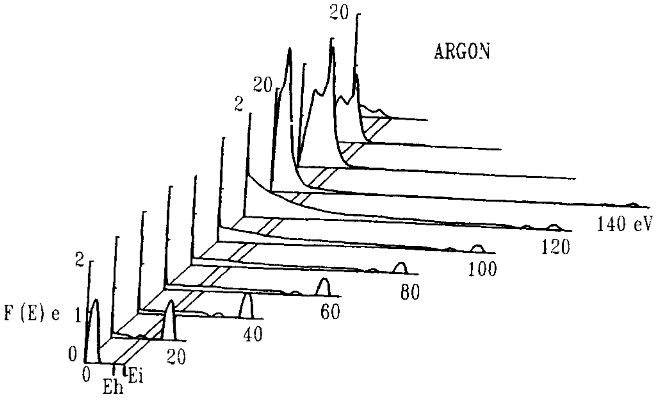

FIGURE 4 The non-equilibrium EEDF in argon in the cathode sheath and negative glow (after W.H. Long, 1979).

Cambridge University Press
978-1-107-41028-2 - Materials Research Society Symposium Proceedings: Volume 165: Characterization of Plasma-Enhanced CVD Processes
Editors: Gerald Lucovsky, Dale E. Ibbotson and Dennis W. Hess
Excerpt
More information

EEDF need not be an equilibrium distribution function such as a Maxwellian.

To examine this approximation we consider the Boltzmann equation in the general form:

$$\frac{df}{dt}(\bar{v},\bar{r},t) + \bar{v}.\nabla_x f + \frac{eE}{m}\nabla_v f = \langle\frac{df}{dt}\rangle_{collisions} \tag{8}$$

The Boltzmann transport equation may be regarded as a continuity equation in six-dimensional phase space (r,v). The first term is the partial time-derivative, the second term represents convection in coordinate-space, the third term is the convection in velocity space and the right-hand side is the collision operator representing all of the possible collision processes. Local field equilibrium occurs when the energy gained in the electric field is immediately balanced by collisions or:

$$\frac{eE}{m}\nabla_v f = \langle\frac{df}{dt}\rangle_{collisions} \tag{9}$$

Therefore this condition will tend to apply in uniform plasmas, at low rf frequencies, and at higher pressures.

LOCAL FIELD NON-EQUILIBRIUM

The local field equilibrium approach will not apply when there are steep concentration or field gradients. As an example, in the cathode sheath the electrons are not in local field equilibrium. The electrons leave the cathode with their lowest energies where the field is actually the highest. The electrons then gain energy from the field much faster than they lose energy by elastic and inelastic collisions. They reach the negative glow with a multi-peaked distribution as the field nears a minimum. Under these conditions the ionization cannot be described by (Townsend) ionization coefficients related to the local electric field, but it must be calculated from a kinetic approach.

Some of the principal approaches that have included treatment of the sheath regions are listed in Table 2. Collisionless plasma sheaths were first analyzed by Tonks and Langmuir [10], who obtained the general plasma-sheath equation and a solution for the sheath that describes a linear field over most of the sheath. These results are confirmed by recent kinetic calculations [11]. The collisionless sheath treatment was extended to rf discharges by Godyak, and by Keller and Pennebaker [12].

As an example of the kinetic approaches, Long [13] considered a one-dimensional sheath by an approach that used a convective characteristic scheme. Considering the dc case for illustration if we divide the Boltzmann equation, eqn (8), by $v_x eE_x$ we obtain