Perturbation of the cathode fall in direct-current glow discharges by particulate contamination

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Particulate (or "dust") contamination of plasma materials processing discharges is known to reduce yields of the product and to perturb electron transport. Dust preferentially accumulates near the cathode sheath-plasma boundary where energetic electrons accelerated in the cathode fall emanate into the negative glow. In this letter, we theoretically investigate the penetration of the electron flux generated in dc cathode falls through the particulate "barriers" formed by dust contamination. We find that at constant current densities, the plasma responds to the reduction in ionization rate coefficients caused by the particulates by increasing the electric field in the cathode fall. In doing so, the cathode fall voltage increases and cathode fall thickness decreases.

Particulates ("dust") in etching and deposition glow discharges are problematic due to the deleterious effects they have on the material being fabricated and the perturbing effects they have on the properties of the plasma. Studies of particulate contamination in both direct-current (dc) and radio-frequency (rf) discharges have been performed by a number of investigators using laser light scattering.[1-10] Although the current densities, gas mixtures, pressures, and source of particulates differed in each of these studies, the common finding was that the particulates are predominantly found at the sheath-plasma boundary (in rf discharges) or at the edge of cathode fall (in dc discharges). This has led to the conclusion that the particulates are negatively charged. The accumulation of particles at the cathode fall-negative glow boundary may be explained by a balance of forces between momentum transfer from Coulomb interactions with ions ("ion drag") which pushes the particles towards the cathode and the electrostatic repulsion of the high electric field in the sheath which pushes the negatively charged heavy particles out of the cathode fall region.[11-13]

The effects that particulates in plasmas have on electron transport are manifested by the charged dust appearing to be massively large multiply charged negative ions, with commensurately large cross sections for momentum transfer. The electron energy distribution (EED) in contaminated plasmas is shifted to lower energies compared to pristine plasmas at the same E/N (electric field/neutral gas number density).[14] This lowers rate coefficients for high threshold events such as electron impact ionization, thereby requiring a higher operational E/N to sustain the plasma. As a result, the current density in nonuniformly contaminated plasmas is channeled around heavily contaminated regions.[13,15,16] High energy ballistic electrons, such as those generated in the cathode fall (CF), can be intercepted and collected by particles since these electrons can have energies greater than the sheath potential of the particle.[13] This is an important effect in a dc CF since particulates accumulate at the location where high energy electrons emerge from the CF and enter the negative glow or positive column. In this paper, we report on a theoretical study of electron fluxes emanating from the CF and penetrating the particulate barrier. We find that the reduction in ionization rates caused by particulate contamination at the edge of the CF is compensated for by larger electric field gradients in the CF (larger CF voltage drop, smaller CF length).

The model we used in this study consists of two linked simulations. The first simulation is a "beam-bulk" model for electron transport in a cathode fall.[17] This model produces a spatially dependent electric field profile and locations of the particulate contamination. The second portion of the model is a Monte Carlo simulation which uses these profiles to generate the EED in the CF while including the effects of particulates. Rate coefficients are then cycled back to the beam-bulk model. These models will be briefly described.

In the beam-bulk model the EED is represented by two components: a monoenergetic beam and a bulk electron swarm. The source of the electron beam is secondary electron emission by ions at the cathode. The local average energy of the beam $\epsilon(x)$ is obtained from

$$\frac{d\epsilon(x)}{dx} = -eE(x) - \sum_i \sigma_i[\epsilon(x)]\Delta\epsilon_i N_i, \tag{1}$$

where E is the local electric field, e is the elementary charge, σ_i is the cross section for a collision with gas species N_i having energy loss $\Delta\epsilon_i$. All beam scattering is assumed to be forward directed. When the electron beam energy falls below the inelastic threshold, its density is added to the bulk plasma. The bulk electron, ion, and excited state densities of the gas are obtained by solving their respective continuity equations. For example, the continuity equation for electrons is

$$\frac{dn_e}{dx} = -\nabla\cdot(v_d n_e - D_e\nabla n_e) + \sum_j (n_e k_j^I + \phi_b \sigma_j^I)\cdot N_j, \tag{2}$$

where v_d and D_e are the electron drift velocity and diffusion coefficient, and ϕ_b is the flux of the electron beam. k_j^I and

σ_j^I are the rate coefficients and cross sections for electron impact ionization with the species having density N_j. k_j^I is obtained from the reduced electric field E/N, and σ_j^I is obtained from the local beam energy. The electric field is obtained by solving Poisson's equation where the self-sustaining E/N in the positive column is used as a boundary condition. The neutral species used in the model are the ground state of argon and the metastable states Ar (4s). The transport coefficients for the bulk plasma species in the CF are obtained from a modified value of E/N which accounts for nonequilibrium of the EED.

The spatial distribution of dust was obtained by solving its continuity equation, $\partial N_D/\partial t = \nabla\cdot v_D N_D = 0$. The drift velocity of the dust is obtained from a balance of electrostatic and ion drag forces[11-13]

$$v_D=\mu_D\cdot\left(-Z'_D\cdot E+\sum_i n_i\sigma_{iD}m_iv_i|v_i|\right) \qquad (3a)$$

$$v_i=\mu_iE-D_{iN}\frac{1}{n_i}\frac{\partial n_i}{\partial z}. \qquad (3b)$$

The ion velocity v_i is found from the mobility μ_i, the diffusion coefficient D_{iN} for ions in the neutral gas, and the electric field E. Z'_D is the shielded charge of the dust particle and σ_{iD} is the cross section for ion momentum transfer (Coulomb interaction) to the dust particle.

The EED in the particulate contaminated CF was obtained from a Monte Carlo–molecular dynamics (MC–MD) hybrid model using the electric field and dust locations from the beam-bulk model. The basic components of the MC–MD model are described in Refs. 14 and 15. In the MC–MD model the trajectories of electrons are tracked using Monte Carlo techniques when they are far from dust particles. Molecular dynamics techniques are used when electrons are within a few Debye lengths of the particle. The particles are assumed to be negatively charged with a sheath potential which is dynamically determined in the model. Electrons approaching a particle with energies less than the sheath potential are deflected by the negative potential of the sheath. Electrons having energies greater than the sheath potential may be collected by the particle.

The spatially varying dust densities were incorporated into the MC–MD model using a modified null cross section technique. When calculating collision frequencies for use in the MC portion of the model, a dust species having a density $N_{\max}$ and an effective cross section corresponding to the Debye sphere surrounding the dust particles were used. When the dust species was randomly selected as a collision partner, another random number was chosen, $r = (0,1)$. If $r < N_D(x)/N_{\max}$, where $N_D(x)$ is the local dust density, then a dust collision occurred. Otherwise, the collision was considered "null." During a dust collision, the equations of motion of the electron are integrated through the sheath of the dust particle until the electron is either collected by the dust or retreats several Debye lengths from the particle.

Typical electric fields obtained from the beam-bulk model in and near the CF of a glow discharge in argon (0.5 Torr, 0.5 mA cm^{-2}) are shown in Fig. 1(a). The calculated CF voltage and thickness in the pristine plasma are 282 V and 0.7 cm, respectively. (The cathode fall thickness is defined here as the distance from the cathode to where the electric field takes on the positive column value.) The location where 1 μm particles accumulate is shown in the inset. The locations where other particles accumulate are shown in Fig. 1(b). Larger particles are found closer to the cathode because the ion drag component of the force is larger. Particles having a specific radius will accumulate at a single location where $v_D = 0$, broadened somewhat by thermal motion. For purposes of demonstration, we chose a distribution of dust for use in the MC–MD model which would form a particulate barrier approximately 0.5 cm wide, which implies a distribution of particle sizes.

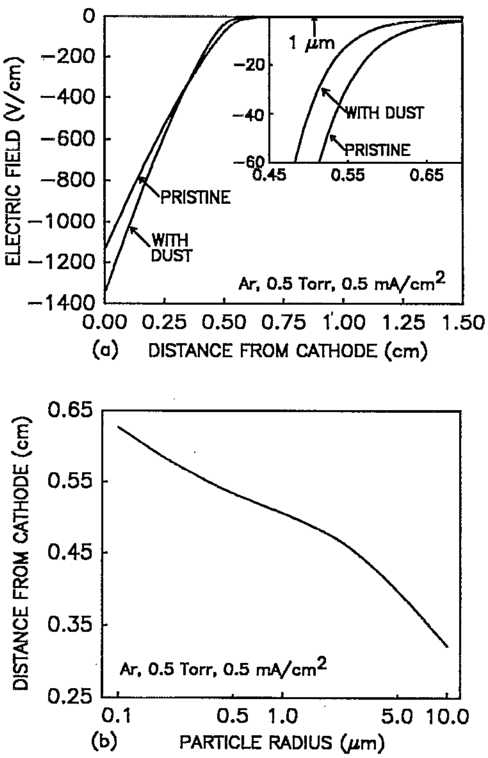

FIG. 1. (a) Electric field near the cathode for 0.5 Torr Ar discharge (0.5 mA/cm^2) with and without particle contamination having density $N_D = 10^7$ cm^{-3}. The location of 1 μm particles is shown by the arrow in the inset. (b) Location of particles as a function of size at the foot of the cathode fall.

The changes in rate coefficients for ionization of ground state argon between a pristine and contaminated CF are shown in Fig. 2 for pressures of 0.5 and 0.8 Torr (dust density $= 10^7$ cm^{-3}). The electric field is also shown. The high energy component of the EED is depressed by intercepting and deflecting collisions of the beam flux with the particles.[13] The result is a depression in the distribution-averaged rate coefficients for ionization in and beyond the dust. The effects are more pronounced at larger values of N_D/N (dust density/gas density). The amount of decrease and extent of the depression in the rate coefficient are greater for the lower pressure case.

If the discharge is operated at a constant current density, the plasma must compensate for the decrease in ion-

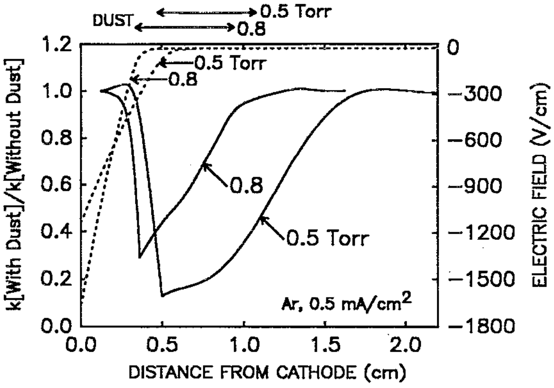

FIG. 2. Cathode fall parameters for 0.5 and 0.8 Torr Ar contaminated glow discharges (0.5 mA/cm^2). The distribution averaged electron impact rate coefficients for ionization in a contaminated cathode fall are shown by the solid lines. The rate coefficients are normalized by their values in a pristine plasma. The electric fields for both pressures are shown by the dashed lines. The extent of the dust is shown by the arrows above the figure.

ization rates at the foot of the CF caused by the dust intercepting the energetic electron flux. This is accomplished by both an increase in the CF voltage and a decrease in the CF thickness, as shown in Fig. 1. The changes in the CF voltage and thickness as a function of pressure are shown in Fig. 3. The locations at which 1 μm particles accumulate are also shown. The changes in voltage and thickness increase with increasing N_D/N. If the particle contamination is nonuniform as a function of position across the cathode, where the cathode fall voltage must be constant, the current density will instead decrease with increasing N_D/N. In a plasma processing environment, the change in excitation rates which result from both the reduction in rate coefficients and decrease in current density could lead to significant nonuniformities in etching or deposition on the substrate.

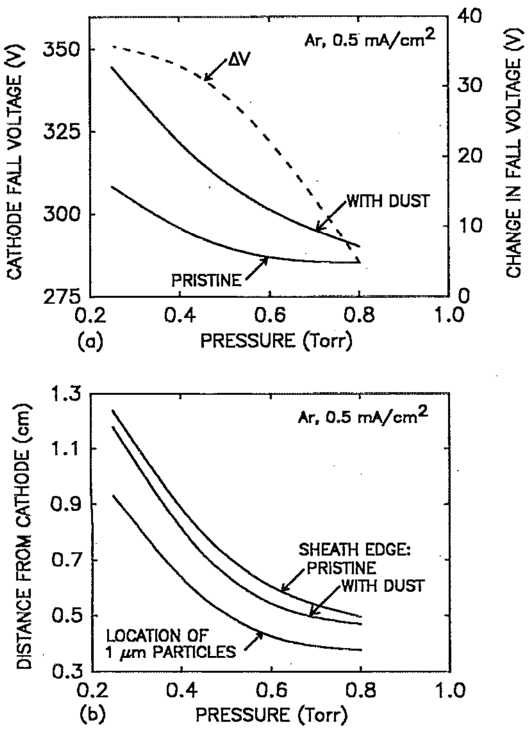

FIG. 3. Cathode fall parameters as a function of Ar pressure (0.5 mA/cm^2) for pristine and contaminated discharges. (a) Cathode fall voltage and the increase in fall voltage caused by contamination; (b) Cathode fall thickness and location of 1 μm particles.

In conclusion, we have theoretically investigated the effects of particle contamination on the cathode fall (CF). We have found that the accumulation of particles at the foot of the CF intercepts the energetic electron flux and reduces excitation rates. If operated at a constant current density, the response of the discharge is to increase the cathode fall voltage and decrease the CF thickness, thereby increasing the electric field in the CF. These effects compensate for the reduction in rate coefficients. The implication for plasma processing discharges is that nonuniformities in particulate contamination, as experimentally observed,[1] can directly lead to nonuniform processing of the substrate.

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