Fast modeling of the low-pressure capacitively coupled radio-frequency discharge based on the nonlocal approach

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The results of modeling a low-pressure capacitively coupled radio-frequency (rf) discharge based on the nonlocal approach are reported. The approximation employed enables fast modeling (FM) of the electron distribution function. The solution of the full problem, which consists of calculation of the electron distribution, rf, and stationary electric fields, and of the plasma density profile, for simple atomic gas takes ~10 min on the IBM PC 486DX2/66. To check the validity of the FM the full scale Monte Carlo modeling was performed. The results of the fast and the full scale modeling are in agreement. © *1996 American Institute of Physics.* [S0003-6951(96)02742-8]

The interest in the complex nature of electron and ion processes in low-pressure radio-frequency (rf) glow discharges has stimulated experimental investigations of the electron distribution function (EDF).[1] Kinetic analyses of the self-consistent motion of electrons and ions in capacitively coupled rf (RFC) discharges have been reported earlier.[2–6] This letter is devoted to the problem of fast simulation of RFC discharge. It is based on the theory developed in Refs. 7 and 8. The fast modeling (FM) for the case of inductively coupled rf discharge was presented in Ref. 5.

Approach description: For simplicity and in order to perform comparison with full (Monte Carlo) kinetic modeling a planar symmetric geometry is considered, but the theory can be easily generalized to more complicated systems. The profiles of electron and ion densities and the region occupied by plasma are schematically shown in Fig. 1. The simplified nonlocal approach used for the FM is valid under the following conditions.[6,7]

(1) The two-term approximation

$$f(x,\mathbf{v},t)=f_0(v,x,t)+f_1(v,x,t)\cos(\theta)$$

holds for the EDF, where θ is the angle between the direction of plasma density gradient and electron velocity $\mathbf{v}$. We can use this approach when discharge length $2L_0$ greatly exceeds electron mean free path λ, and inequality $\nu \gg \nu^*$ holds, where ν is a transport electron collision frequency and ν^* is an inelastic collision frequency.

(2) We suppose that discharge frequency satisfies $\omega \gg \nu^*$. Therefore, EDF is practically stationary during the rf field period T.

(3) The electron plasma frequency ω_{0e} exceeds max $(\sqrt{\nu\omega},\omega)$over the whole plasma volume. It means that the quasineutrality condition $n_e \cong n_i$ may be used in the plasma phase, at the points and in the moments where and when (in the sheath) electrons are actually present. In coordinates $\{x,t\}$, the plasma phase corresponds to the single-hatched region [see Fig. 1(b)]. Since $\omega_{0e} \gg$ max$(\sqrt{\nu\omega},\omega)$the total current in the plasma phase coincides with electron current.[6]

(4) For typical plasma densities the inequality $\omega_{0i} \ll$ max$(\sqrt{\nu_i\omega},\omega)$ is valid, where ω_{0i} is an ion plasma frequency, and ν_i is an ion–neutral collision frequency. Consequently, the ion displacement during the field period is much lower than the sheath thickness $L_{\mathrm{sh}}=L_0-L_p$; so, the ion density profile is stationary.[6]

(5) The discharge space consists of two regions: the region of quasineutral plasma, where $n_e \cong n_i$, and the region of ionic space charge. The region occupied by the plasma appears to oscillate between the electrodes. The applied voltage is screened by the ionic space charge at the plasma periphery [Fig. 1(a)]. The electron density exponentially decreases within the sheath. The width of this transitional region be-

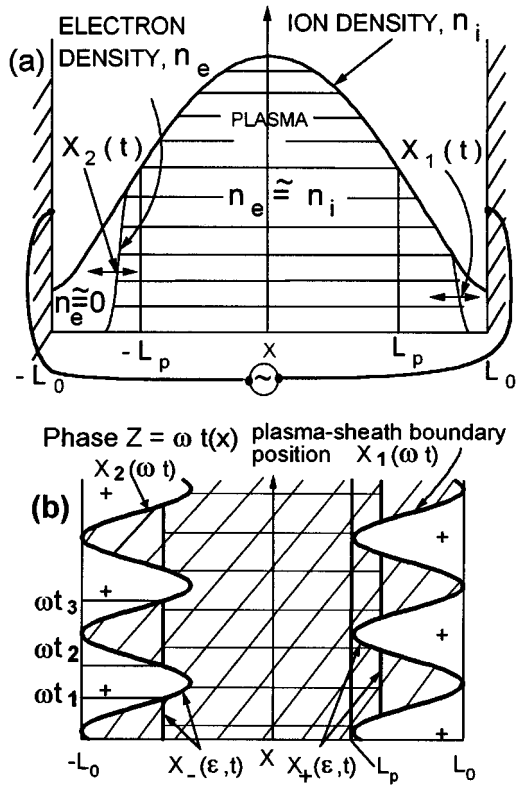

FIG. 1. (a) Sketch of the RFC discharge. (b) Sketch of the plasma motion and region of electron motion.

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tween the plasma and the ionic space charge is of the order of the Debye radius. Usually, the amplitude of applied voltage is much larger than the electron temperature (divided by electron charge). Therefore, the Debye radius is small in comparison to $L_{\rm sh}$.[6] This sharp boundary corresponds to the rigid potential ''walk,'' which specularly reflects the electrons [see Fig. 1(b)]. The plasma–sheath boundary motion as a function of ωt corresponds to the curves $X_{1,2}(\omega t)$ [see Fig. 1(b)]. At any point of the sheath [within $L_p<|x|<L_0$, Fig. 1(a)] the whole field period is to be divided into two parts. During the first part the electrons are absent [$t_1<t<t_2$, Fig. 1(b)] and during the second one $n_e \cong n_i$ holds. In other words, during the first part of the field period at any given point of the sheath, the ionic space-charge phase occurs, while during the second one it is replaced by the plasma phase.

(6) The stationary ambipolar field $\overline{E(x)}$which traps the electrons exists only in the plasma phase [single-hatched region in Fig. 1(b)]. Thus, the electric field in plasma ($|x|<L_p$) and in the plasma phase the sheath can be divided into an oscillatory part $\widetilde{E}(x,t)$, which accounts for ordinary ohmic heating, and a dc part $E(x)$ which does not perform any work. The proposed field dividing in the plasma is represented by

$$E(x,t)=\widetilde{E}(x,t)+\overline{E(x)}.$$

Here, $\overline{E(x)}$ is obtained from

$$\overline{E(x)}=\frac{\omega}{2\pi}\int_0^{\omega/2\pi}\widetilde{E}(x,t)dt=-\frac{d\Phi}{dx}.$$

Within the sheath, the time averaging of this equation has to be performed over the plasma phase–time interval (t_3-t_2) [see Fig. 1(b)].

(7) It is convenient to introduce a new variable—a total electron energy $\epsilon=u+e\Phi$, where u is a kinetic electron energy into the time-averaged electron kinetic equation.[6,7] Electrons are trapped by potential Φ. When the energy relaxation length λ_ϵ exceeds L_0, the total electron energy is practically conserved during its displacement over the available region between the turning points $X_-(\epsilon,t), X_+(\epsilon,t)$[the double-hatched region in Fig. 1(b)]. The energy relaxation length can be estimated as $\lambda_\epsilon \sim \sqrt{\lambda\lambda^*/3}$ at the EDF tail (λ^* is a mean free path for inelastic collisions).

When conditions (1)–(7) are applicable, a single isotropic function $F_0(\epsilon)$ depending solely on a total electron energy ϵ related to x as $\epsilon=u+e\Phi(x)$ proves to be suitable for an adequately accurate description of electron kinetics. In comparison to $F_0(\epsilon)$ the time- and coordinate-dependent parts of the EDF are small corrections of the order of (ν^*/ω) and $(L_0/\lambda_\epsilon)^2$.

Electron kinetic equation: For the FM the function $F_0(\epsilon)$ which is calculated from the spatially and temporally averaged kinetic equation is used,[6,7]

$$\frac{d}{d\epsilon}\left(\overline{\upsilon D_\epsilon(u,x)}\,\frac{dF_0(\epsilon)}{d\epsilon}\right)$$

$$=\sum_k \overline{\upsilon\,\nu_k^*(u)}F_0(\epsilon)-\sum_k \overline{\upsilon\,\nu_k^*}(\epsilon+\epsilon_k^*)F_0(\epsilon+\epsilon_k^*), \quad (1)$$

where the energy diffusion coefficient is given by

$$\upsilon D_\epsilon(u,x)=e^2\upsilon^2\nu\widetilde{E}_0^2(x)/[6(\omega^2+\nu^2)], \quad (2)$$

and $\nu(u)$ and $\nu_k^*(u)$ are elastic transport and inelastic collision frequencies, respectively, and $\epsilon_k^*$is an inelastic collision threshold. $\widetilde{E}_0(x)$ is an amplitude of the oscillatory field defined by $\widetilde{E}(x,t)=\widetilde{E}_0(x)\exp(-i\omega t)$. The space–time averaging is to be performed according to

$$\overline{G(u,x)}\equiv\overline{G(\epsilon)}$$

$$=\frac{1}{2L_0T}\int_{0X_-}^{TX_+(\epsilon,t)}\int_{(\epsilon,t)}G[\epsilon-e\Phi(x),x]dx'dt. \quad (3)$$

The spatially averaged coefficients in Eq. (1) depending only on ϵ account for heating of electrons in rf electric field and inelastic energy losses. The complete set of equations for electrons comprises[6,7] the kinetic equation (1), and two expressions: one for the plasma density combined with quasineutrality condition,

$$n_i(x)=n_e(x)=\frac{4\pi}{m}\int_{e\Phi(x)}^{\infty}F_0(\epsilon)\left(\frac{2}{m}[\epsilon-e\Phi(x)]\right)^{1/2}d\epsilon,$$

$$\Phi|_{x=0}=0, \quad \left.\frac{d\Phi}{dx}\right|_{x=0}=0, \quad (4)$$

and another for the electron current,

$$j_0=-\frac{8\pi e^2\widetilde{E}_0(x)}{3m^2}\int_{e\Phi(x)}^{\infty}\upsilon\frac{\epsilon-e\Phi(x)}{\nu+i\omega}\frac{dF_0}{d\epsilon}\,d\epsilon. \quad (5)$$

The ion density profile is determined in the standart mobility approach with the source term which is determined by $F_0(\epsilon)$ and $\Phi(x)$. The dc field $\Phi(x)$ is to be found from Eq. (4), and the rf field from the electron current conservation (5). To perform the FM it is easier to prescribe a current density $j_0\exp(i\omega t)$ instead of amplitude of the applied voltage. It should be noted that the field division proposed above allows one to avoid the solution of the Poisson equation in plasma, requiring the cumbersome calculation of small difference $[n_e(x,t)-n_i(x,t)]$ with high accuracy. Thus, the field division together with the approximation of total energy conservation are the main points of the nonlocal theory briefly considered here. These particular assumptions make the simulation of electron kinetics fast.

Results: (1) To demonstrate the validity of nonlocal approach and the method of field division the following simulations are performed. For the reasons of comparison the EDF values calculated by both FM and Monte Carlo (MC) methods are presented (jointly in Fig. 2). The model He-like gas is considered. Elastic collision frequency has been assumed energy independent, 5×10^8 s^{-1}. Inelastic collisions are defined by the cross section: 1.41×10^{-17} $(\epsilon-\epsilon^*)$ cm^2 (excitation with a threshold energy $\epsilon^*=20$ eV). The Poisson equation and electron kinetic equation have been solved self-consistently using the MC techniques. Since we intended to analyze only electron kinetics we restricted ourselves in these simulations to the case of fixed ion density (Fig. 3). The following set of discharge parameters for the MC simulation was introduced: applied voltage 62 V; discharge frequency $\omega=2\pi\times15\times10^6$ rad s^{-1}; $L_0=2$ cm; pressure p

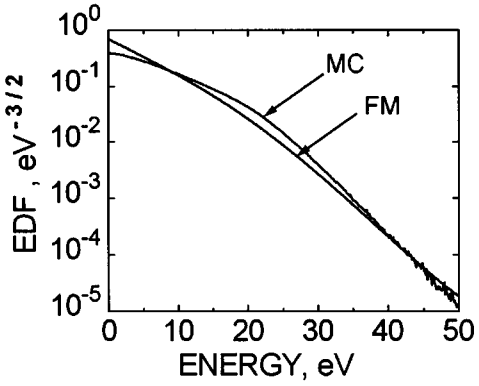

FIG. 2. Comparison between EDF calculated in the nonlocal approach (marked as FM) and by Monte Carlo technique (marked as MC).

$=0.01$ Torr. The resulting EDF, which practically does not exhibit any variation with time during rf period, is marked by ''MC'' in Fig. 2. Current density $j_0=0.35$ mA/cm^2 from MC simulation has been taken for FM. The agreement between FM and MC EDF seems reasonable.

Values of all fields given by the FM also prove to be in reasonable agreement with the full-scale modeling. The sine and cosine Fourier harmonics $\widetilde{E}_{\sin}(x)$ and $\widetilde{E}_{\cos}(x)$ of the rf field have been calculated in the MC simulation. The amplitude of oscillatory field given by MC simulation corresponds to

$$E_0(x)=\sqrt{[\widetilde{E}_{\sin}(x)]^2+[\widetilde{E}_{\cos}(x)]^2}$$

in the central part of discharge ($|x|<L_p$). The obtained value differs from that calculated by FM (5) by less than 5%. The difference between the time-averaged part of the rf field obtained by MC and the gradient of the potential field (4) obtained by FM does not exceed 5% (comparison has been made in the region $|x|<L_p$). The discharge rf voltage is determined mainly by the strong ion space-charge field. And since the resulting amplitude of applied voltage obtained by FM is in agreement with the one utilized in the MC (relative difference is about $\sim$10%), we can conclude that the values of ionic space-charge fields obtained by FM and MC simulations are in agreement, too. The difference of order of electron temperature can be attributed to the used in the FM

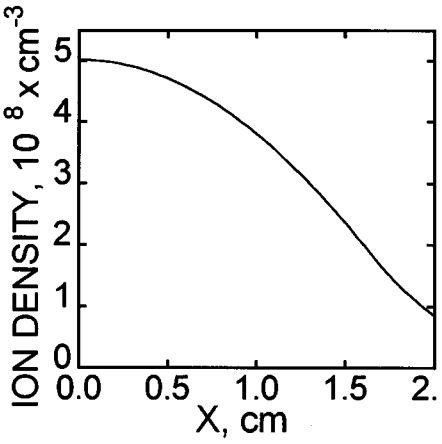

FIG. 3. The ion density profile that has been used for simulations.

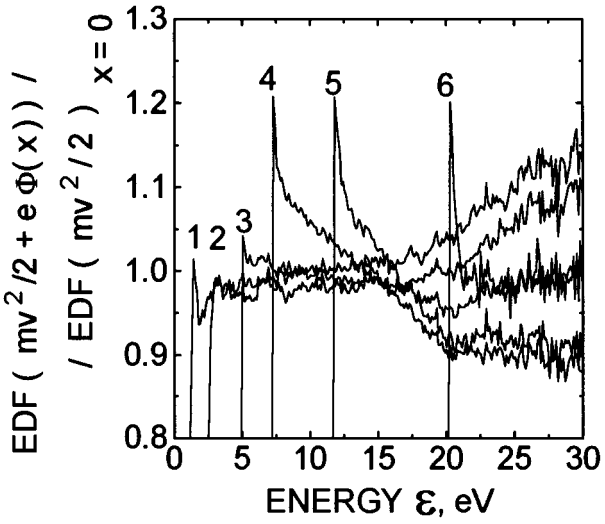

FIG. 4. The ratios of the shifted EDFs (calculated at different spatial points) to the EDF calculated at the center of the discharge: (1) $x=0.69$ cm; (2) $x=1.0$ cm; (3) $x=1.35$ cm; (4) $x=1.5$ cm; (5) $x=1.67$ cm; (6) $x=1.84$ cm. The EDF is equal to zero at $\epsilon<e\Phi(x)$.

approximation of zero Debye radius. Thus, the dividing of electric field into three independent parts—the dc and oscillatory fields in the plasma phase and strong field in the ionic space-charge phase—proves to be reasonably grounded and efficient.

In Fig. 4 MC EDFs in different spatial points are shown. These functions, which are normalized by the density at the corresponding spatial points, are shifted along the energy axis by the plasma potential $e\Phi(x)$ and are divided by the EDF calculated at the discharge center. These ratios are close to unity up to energies $\approx$35–40 eV (the difference, less than 20%, is very small compared to EDF variation, which is nearly 10^5). This indicates that the EDF depends practically only on ϵ. Consequently, the EDF is nonlocal. The value of $\lambda_\epsilon=2$ cm at $\epsilon=30$ eV. It corresponds to accuracy of the nonlocal approach of order of $(L_p/\lambda_\epsilon)^2\sim 0.2$.

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