Simulation of the secondary-electron distribution function by a Monte Carlo method

V. S. Malinovsky
Institute of Thermophysics, Russian Academy of Sciences, Novosibirsk, 630090, Russia

A. V. Vasenkov
Novosibirsk State University, Novosibirsk, 630090, Russia

(Received 8 December 1993)

A Monte Carlo (MC) direct simulation method for calculating the stationary electron distribution function (EDF) in an electron-beam plasma was developed. The EDF calculations in argon and molecular nitrogen were done. A good agreement of the results of the EDF simulation by the MC method with those obtained using the Boltzmann equation was shown.

PACS number(s): 52.20.Fs

I. INTRODUCTION

The electron distribution function (EDF) as a function of electron energy and position is one of the most important characteristics of the interaction between an electron beam and gas medium. There being a great number of studies dealing with the interaction between electrons and gas, there are still very few reported data on the EDF with energy values above the ionization threshold, and specifically on the EDF as a function of position [1–3]. It becomes common practice to determine the EDF using either the Boltzmann equation or different modifications of the Monte Carlo (MC) method. Traditionally, quasistationary homogeneous conditions are considered [4]. Stated differently, the electron energy distribution function was assumed to be the same in each point of space, hence the motion of electrons in space was not analyzed.

The present paper reports a MC direct simulation method for calculating the stationary distribution function of electrons generated by a high-energy electron beam in a gas of homogeneous density. Particular calculations have been made for argon and molecular nitrogen. The results of a direct simulation have been compared with those obtained by solving the Boltzmann equation [5,6].

II. THE MONTE CARLO METHOD ALGORITHM

As a high-energy electron beam passes through a gas medium, a low-temperature and weakly ionized plasma swarm forms around the beam, resulting from molecule ionization and scattering processes. The rate of excited particle formation in plasma was determined by the EDF. To calculate the EDF and excitation rates of molecules of the homogeneous density gas, we suggest employing the MC direct simulation method to be described as follows.

In the first stage a spatial form of a primary electron beam was set specifying the distribution of secondary-electron sources. The energy of each electron in the beam was considered to be constant, since inelastic scattering of primary electrons was neglected. The energy of each secondary electron resulting from ionization was chosen according to the secondary-electron spectrum. The energy range of secondary electrons from the lowest threshold value of electron excited states to $(E-I)/2$, where E is the primary electron energy and I is the ionization potential of molecules, was considered. To set positions of secondary-electron sources a conventional technique was used, while for their energies the acceptance-rejection method [7] was employed.

Given the initial conditions described above, the motion of each secondary electron was simulated. Their total number was originally equal to the number of sources. The generated secondary electron was in free motion until it collided with a molecule. The free run length was found by the formula [8]

$$l=-\frac{1}{n_g\sigma_j(e)}\ln(W)\ ,$$

where n_g is the gas density, $\sigma_j(e)$ is the cross section of the jth scattering process with the electron energy e, and W is a random number.

The type of collision for each electron was chosen according to the distribution $\sigma_j(e)/\sigma_t(e)$, where $\sigma_t(e)=\sum_j\sigma_j(e)$ is total cross section with the electron energy e. Elastic scattering, ionization, and excitation of electron states of molecules were taken into account. All cross sections were considered as being spatially uniform. Electron-electron and electron-ion collisions, multistage ionization, and impacts of the second kind, as well as energy losses of electrons under elastic scattering on molecules, were neglected. If the chosen collision type resulted in ionization, the procedure of generating another secondary electron would be employed. Its energy was determined according to the secondary-electron spectrum over the range from the minimum energy threshold of electron excitation state to the energy $(e-I)/2$ where e is the energy of an impinging electron. Positions of the generated electron were considered coincident with those where ionization occurred.

Subsequent to the choice of the free run length, the escape of the electrons from the simulation region was considered. The electrons that went out from the simulation domain, as well as those with the energies below the

minimum energy threshold of electron excitation state of molecules, were eliminated from consideration. The above procedure was repeated until the stationary distribution function was determined.

III. EXCITATION RATE OF MOLECULES AND EDF IN ELECTRON-BEAM PLASMA

The presented model was used to determine the spatial dependencies of excitation rates of molecule electron states and the electron energy distribution function in each point of space. The dependence of the excitation rate of the jth electron state on the distance from the center of primary electron beam was found from the following expression:

$$F_j(R_i)=n_g\sigma_j(E)v_b n_b(R_i)+n_g\sum_k \sigma_j(e_k)v_k n(R_i,v_k)\ , \tag{1}$$

where R_i is the distance from the center of the primary electron beam to the center of the ith cell, $n_b(R_i)$ is the density of primary electrons in the ith cell, and $n(R_i,v_k)$ is the distribution function of the secondary electrons in the ith cell. The first term in (1) represents the contribution of primary electrons to the excitation rate of the jth state, while the second one describes the contribution of secondary electrons. The second term in (1) exhibits the summation over energies of electrons in the ith cell.

The energy distribution function of electrons arising from ionization of molecules is also one of the most notable characteristics of plasma. In our model, information about the electron energy distribution function of secondary electrons may be obtained using the energy dependence of the number of electrons with the energies exceeding $e_{\min}$ in the finite volume. The number of such secondary electrons in a cylinder of radius R and length L around the primary electron beam is determined by the expression

$$N_{\rm sec}(e_{\min})=2\pi L\sum_{l,0<r_l<R\,k,e_{\min}<e_k<e_{\max}} n(r_l,v_k)\ , \tag{2}$$

where $e_{\max}$ is the maximum possible value of the secondary-electron energy.

The foregoing covers general aspects of the proposed method. To do particular calculations, we have chosen molecular nitrogen and argon as gas media. The reason is that, on the one hand, there is ample and rather complete information about electron scattering cross sections, and, on the other hand, these gases are being extensively studied in atmospheric physics and are also being widely used in plasma-chemical deposition of thin films in microelectronics.

For our calculations we used the following data on cross sections: for N_2, the ionization cross section [9], the electron state excitation cross sections [10,11], and the momentum transfer cross section [12]; for Ar, the ionization cross section [9], the electron state excitation cross sections [13,14], and the momentum transfer cross section [15]. For N_2 the secondary-electron spectrum was taken from [16,17], and for Ar from [18].

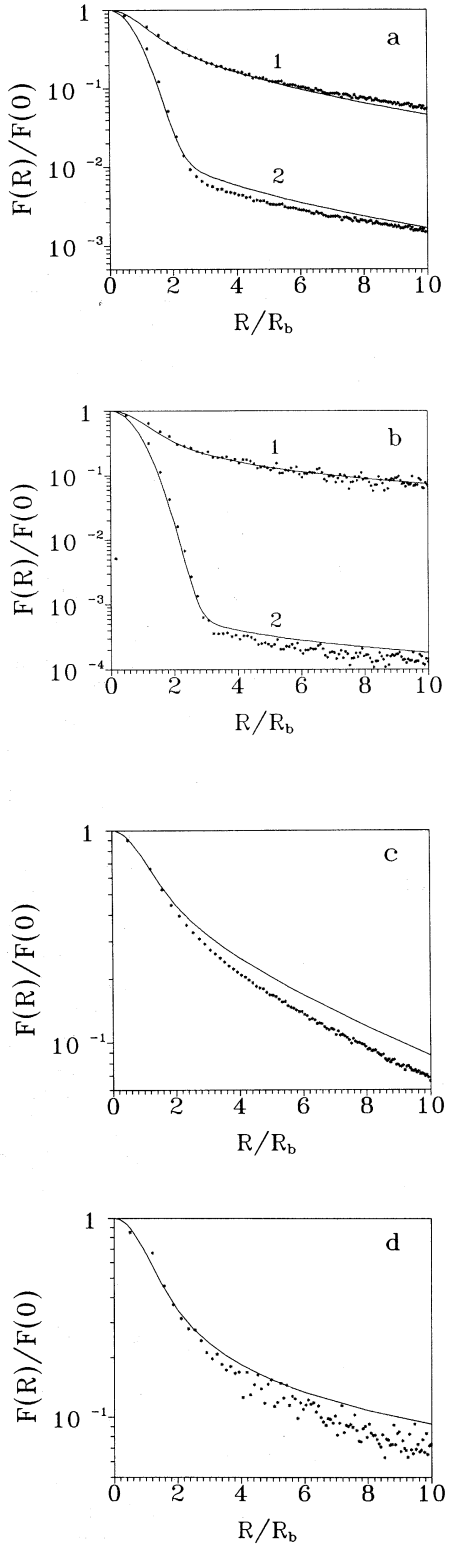

FIG. 1. Radial dependencies of the excitation rates of the electron states and the ionization rate in N_2 at $E=5$ keV. (1) Contribution of secondary electrons. (2) Total contribution. Solid lines, Boltzmann equation. Points, MC. (a) Ionization rate, $R_b=0.32$ cm, $n_g=9\times10^{14}$ cm^{-3}; (b) ionization rate, $R_b=0.25$ cm, $n_g=8.7\times10^{13}$ cm^{-3}; (c) excitation rate of state $C^3\Pi_u$, $R_b=0.32$ cm, $n_g=9\times10^{14}$ cm^{-3}; (d) excitation rate of state $C^3\Pi_u$, $R_b=0.25$ cm, $n_g=8.7\times10^{13}$ cm^{-3}.

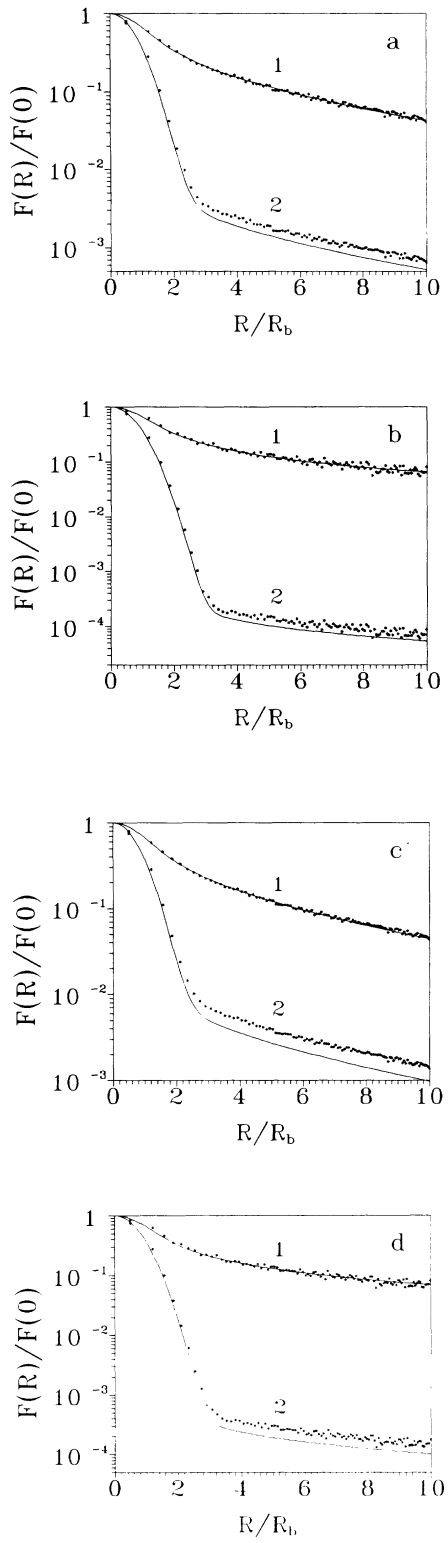

FIG. 2. Radial dependencies of the excitation rates of the electron states and the ionization rate in Ar at $E=5$ keV. (1) Contribution of secondary electrons. (2) Total contribution. Solid lines, Boltzmann equation. Points, MC. (a) Ionization rate, $R_b=0.32$ cm, $n_g=9\times10^{14}$ cm^{-3}; (b) ionization rate, $R_b=0.25$ cm, $n_g=8.7\times10^{13}$ cm^{-3}; (c) excitation rate of state $3d_{1/2}$, $R_b=0.32$ cm, $n_g=9\times10^{14}$ cm^{-3}; (d) excitation rate of state $3d_{1/2}$, $R_b=0.25$ cm, $n_g=8.7\times10^{13}$ cm^{-3}.

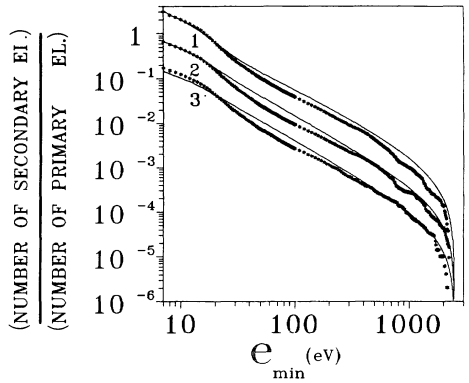

FIG. 3. The normalized number of secondary electrons in N_2, in a cylinder of the radius $R=10R_b$, at the energy exceeding some energy value e_{min}, $E=5$ keV: (1) $R_b=0.32$ cm, $n_g=9\times10^{14}$ cm^{-3}; (2) $R_b=0.26$ cm, $n_g=2.7\times10^{14}$ cm^{-3}; (3) $R_b=0.25$ cm, $n_g=8.7\times10^{13}$ cm^{-3}. Solid lines, Boltzmann equation. Points, MC.

To elucidate the possibilities of the proposed method, we present the calculation results of radial dependencies of ionization rates in N_2 [Figs. 1(a) and 1(b)] and Ar [Figs. 2(a) and 2(b)], as well as excitation rates of the electron states N_2: $C^3\Pi_u$ [Figs. 1(c) and 1(d)] and Ar: $3d_{1/2}$ [Figs. 2(c) and 2(d)] at different values of the gas density. The form of the primary electron beam (the beam radius R_b) was set to be Gaussian. The energy of the electron beam was taken at 5 keV. The figures present the profiles of the electron state excitation and ionization rates solely by secondary electrons, and those of the total excitation by both secondary and primary electrons. Solid lines show the results of calculations of the corresponding quantities on the basis of the Boltzmann equation [5,6]. It should be noted that the state $C\,^3\Pi_u$ of a molecule in N_2 is practically not excited by high-energy electrons of the beam, thus only rates of excitation by secondary electrons were compared.

As can be seen from the figures, the form of spatial dis-

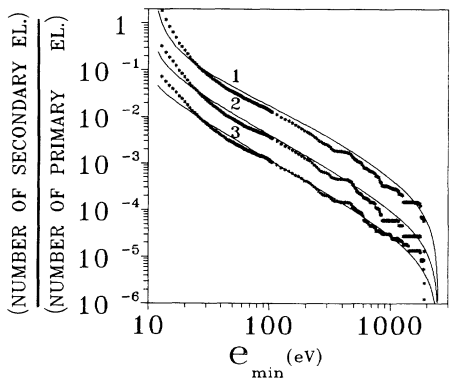

FIG. 4. The normalized number of secondary electrons in Ar, in a cylinder of the radius $R=10R_b$, at the energy exceeding some energy value e_{min}. Designations are the same as in Fig. 3.

tribution of secondary electrons is much more even than that of primary electrons of the beam with the Gaussian profile. This fact is essential for the growth of thin films from gas mixtures excited by an electron beam where the homogeneity of the excited flow on the substrate is one of the problems.

Figures 3 and 4 show the energy dependencies of the normalized number of secondary electrons with the energies exceeding e_{min} [Eq. (2)] to the quantity of primary electrons in the beam at different densities in N_2 (Fig. 3) and Ar (Fig. 4). As above, for comparison the results obtained on the basis of the Boltzmann equation [5,6] are shown. It is seen from the figures that the behavior of dependencies is practically invariant with the increase in the gas density value. Note that at high densities the total number of secondary electrons exceeds the quantity of primary electrons. Taking into account that excitation cross sections of different states of molecules (atoms) decrease with the increase in energy from 100 eV and on, one can arrive at the conclusion that secondary electrons make an essential, if not a greater, contribution to electron state excitation, ionization, and dissociation of molecules.

The rather good agreement between the results of direct simulation of the EDF and those obtained using the Boltzmann equation points to the adequacy of the proposed model and the correctness of the calculations. The above model may be employed to perform calculations in more complicated cases, in particular under heterogeneous gas density.

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