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Drift Velocities of Electron Swarms in Methane : A Multi-Term Boltzmann Equation Analysis

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Abstract

The drift velocities deduced from the flight distance spectrum (FDS) and the arrival time spectrum (ATS) of an electron swarm in the methane gas are calculated at E/p_0 values from 1 to 300 Vcm^{-1} $Torr^{-1}$. In the method for solving the equations for the FDS and ATS analyses, a multi-term (six-term) spherical harmonic expansion technique is employed. The result shows the differences in values of the various drift velocities: the center-of-mass drift velocity W_r, the mean drift velocity W_v, the drift velocity for the steady-state-Townsend V_d and the mean arrival time drift velocity W_m, at high E/p_0 values larger than 50 Vcm^{-1} $Torr^{-1}$. In particular, with focusing on the values of W_m, a comparison of the validity and accuracy of both the ATS method and the FDS method is also made, and it is shown that the ATS analysis is an effective and exact method to deduce the experimental time-of-flight (TOF) parameters.

1. Introduction

Exact knowledge on the drift velocity of electron swarms is essentially important since it greatly helps us to determine electron collision cross sections and to analyze the discharge plasmas now applied in plasma processing, plasma displays, gas lasers, e-beam switches, discharge lamps, X-ray tube, gas insulation and other important areas of modern technology.

One of the methods to represent the behaviour of electron swarms and to derive the drift velocities or other parameters such as the Townsend first ionisation coefficient and diffusion coefficients is that of the Boltzmann equation.

In conventional investigation by using the Boltzmann equation, the so-called time-of-flight (TOF) parameters, which are defined as the time derivatives of the spatial moments of electron density distribution, are obtained as reported by many authors (e.g. Huxley and Crompton 1974, Tagashira et al 1977, Kitamori et al 1980, Kumar et al 1980, Pitchford et al 1981 and Segur et al 1983). However, in usual experiments for the time and space evolution of electron swarms, the arrival time spectrum of a swarm is observed at constant positions in the field direction in the drift space, thus the swarm parameters directly obtained by those experiments are not the

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conventional TOF parameters when ionisation and/or attachment are present. The authors have recently presented a new method in which the swarm parameters defined as the space derivatives of the moments of the arrival time are deduced (Kondo and Tagashira 1990). This method has made it possible to calculate the swarm parameters which are defined consistently with the experiment, such as the mean arrival time drift velocity W_m.

In the present paper the drift velocities of electron swarms defined by the different principles in methane are calculated, and the relations between the swarm parameters by the conventional method (hereafter referred to as FDS ; flight distance spectra method) and by the method of arrival time spectra (hereafter referred to as ATS) are examined at high values of E/p_0 above 100 Vcm^{-1} $Torr^{-1}$. The computation for the both methods are performed by using the multi-term (six-term) method by an amalgamated procedure of the conventional two-term expansion technique and Galerkin technique (Yachi et al 1988).

2. Method of calculation

2.1 Boltzmann equation

The distribution function at time t and position z in the direction parallel to the electric field E should satisfy the Boltzmann equation as follows :

$$\frac{\partial f}{\partial t}+v_z\frac{\partial f}{\partial z}+\frac{eE}{m}\frac{\partial f}{\partial v_z}+Jf=0 \tag{1}$$

where f has been integrated over the lateral direction to the electric field as

$$f(\boldsymbol{v},z,t)=\iint f(\boldsymbol{v},\boldsymbol{r},t)dxdy \tag{2}$$

Here, e and m are respectively the electronic charge and mass, J is the collision operator, and $\boldsymbol{v}$ is the electron velocity.

2.2 FDS method

In the FDS method, the distribution function $f(\boldsymbol{v},z,t)$ is expanded in the form (3) and the continuity equation can be represented as equation (4) (Tagashira et al 1977).

$$f(\boldsymbol{v},z,t)=\sum h^K(\boldsymbol{v},t)\cdot\left(-\frac{\partial}{\partial z}\right)^K n(z,t) \tag{3}$$

$$\frac{\partial n(z,t)}{\partial t}=\sum \omega^{(K)}(t)\cdot\left(-\frac{\partial}{\partial z}\right)^K n(z,t) \tag{4}$$

where $(-\partial/\partial z)^K n(z,t)$ represents the spatial density gradient along the z axis at t and z.

Substituting (3) and (4) into (1) gives a series of equations for $h^K(\boldsymbol{v})$ independent of t in the so-called hydrodynamic regime (Kumar et al 1980) as follows.

$$\left(\frac{eE}{m}\frac{\partial}{\partial v_z}+\omega^{(0)}+J\right)h^0(\boldsymbol{v})=0 \qquad \text{for } K=0$$

$$\left(\frac{eE}{m}\frac{\partial}{\partial v_z}+\omega^{(0)}+J\right)h^K(\boldsymbol{v})=v_z h^{K-1}(\boldsymbol{v})-\sum_{J=1}^{K}\omega^{(J)}h^{K-J}(\boldsymbol{v}) \qquad \text{for } K\geq 1 \tag{5}$$

Here, $\omega^{(K)}$ $(K=0,1,2)$ are given by

$$\omega^{(0)}=\int vNq_{ia}(v)h^0(\boldsymbol{v})d\boldsymbol{v} \quad (=R_{ia}) \tag{6}$$

$$\omega^{(1)}=\int v_z h^0(\boldsymbol{v})d\boldsymbol{v}-\int vNq_{ia}(v)h^1(\boldsymbol{v})d\boldsymbol{v} \quad (=W_r), \tag{7}$$

$$\int v_z h^0(\boldsymbol{v})d\boldsymbol{v}=W_v$$

$$\omega^{(2)}=-\int v_z h^1(\boldsymbol{v})d\boldsymbol{v}+\int vNq_{ia}(v)h^2(\boldsymbol{v})d\boldsymbol{v} \quad (=D_L) \tag{8}$$

where $q_{ia}(v)$ denotes $q_i(v)-q_a(v)$, $q_i(v)$ is the ionisation cross section and $q_a(v)$ is the attachment cross section, and $\omega^{(K)}$ $(K=0,1,2)$ are equivalent to the effective ionisation frequency R_{ia}, the center of mass drift velocity W_r and the longitudinal diffusion coefficient D_L, respectively. W_v is the drift velocity defined as the mean velocity of the electrons in a swarm.

2.3 ATS method

For the analysis of ATS, the distribution function $f(\boldsymbol{v},z,t)$ can be expanded in the form (9) and the transport equation may be written as equation (10) (Kondo and Tagashira 1990).

$$f(\boldsymbol{v},z,t)=\sum g^K(\boldsymbol{v},z)\cdot\left(-\frac{\partial}{\partial t}\right)^K n(z,t) \tag{9}$$

$$\frac{\partial n(z,t)}{\partial z}=\sum \alpha^{(K)}(z)\cdot\left(-\frac{\partial}{\partial t}\right)^K n(z,t) \tag{10}$$

where $(-\partial/\partial t)^K n(z,t)$ represents the time derivatives of electron number density at t and z. It is noted that z in equations (3) and (4) is replaced by t in equations (9) and (10).

Taking the successive moments of the time on (10), we have the alpha-parameters (Kondo and Tagashira 1990) :

$$\alpha^{(0)}=\frac{d(\log N(z))}{dz}=\alpha_T \tag{11-a}$$

$$\alpha^{(1)}=\frac{d\langle t\rangle}{dz}=\frac{1}{W_m} \tag{11-b}$$

$$\alpha^{(2)}=\frac{d\langle T^2\rangle}{dz} \tag{11-c}$$

$$N(z)=\int n(z,t)dt$$

where $T=t-\langle t\rangle$, $\langle t\rangle$ is the mean arrival time of a swarm at fixed positions, $\alpha^{(0)}$ represents the Townsend first ionisation coefficient α_T and $\alpha^{(1)}$ is identified as the reciprocal of the mean arrival time drift velocity W_m. $N(z)$ is the number density at z of the steady-state-Townsend (SST) experiment. The diffusion modified drift velocity (V_d) for SST experiment is obtained in the ATS analysis as,

$$V_d=\int v_z g^0(\boldsymbol{v})d\boldsymbol{v} \tag{12}$$

Substituting (9) and (10) into (1), similarly to the FDS method, gives a series of equations for $g^K(\boldsymbol{v})$ independent of z at a long enough distance from the cathod as follows.

$$\left(\frac{eE}{m}\frac{\partial}{\partial v_z}+\alpha^{(0)}v_z+J\right)g^0(\boldsymbol{v})=0 \qquad \text{for } K=0$$

$$\left(\frac{eE}{m}\frac{\partial}{\partial v_z}+\alpha^{(0)}v_z+J\right)g^K(\boldsymbol{v})=g^{K-1}(\boldsymbol{v})-v_z\sum_{J=1}^{K}\alpha^{(J)}g^{K-J}(\boldsymbol{v}) \quad \text{for } K\geq 1 \tag{13}$$

2.4 Spherical harmonics expansion

To solve the hierarchy of equations (5) and (13) the Legendre polynomials of spherical harmonics expansion can be employed as in the conventional manner.

$$h^K(\boldsymbol{v})=\sum_n h_n^K(v)P_n(\cos\theta_v) \tag{14}$$

$$g^K(\boldsymbol{v})=\sum_n g_n^K(v)P_n(\cos\theta_v) \tag{15}$$

Substituting equations (14) and (15) into (5) and (13) gives a series of equations for h_n^K and g_n^K, the nth-order distributions for $K=0,1,2\cdots\cdots$, respectively as follows.

$$\frac{eE}{m}\left[\frac{n}{2n-1}\left(\frac{d}{dv}-\frac{n-1}{v}\right)h_{n-1}^0+\frac{n+1}{2n+3}\left(\frac{d}{dv}+\frac{n+2}{v}\right)h_{n+1}^0\right]+J_n h_n^0=\omega^{(0)}h_n^0 \qquad \text{for } K=0$$

$$\frac{eE}{m}\left[\frac{n}{2n-1}\left(\frac{d}{dv}-\frac{n-1}{v}\right)h_{n-1}^K+\frac{n+1}{2n+3}\left(\frac{d}{dv}+\frac{n+2}{v}\right)h_{n+1}^K\right]+J_n h_n^K$$

$$=\sum_{J=1}^{K}\omega^{(J)}h_n^{K-J}-v\left(\frac{n}{2n-1}h_{n-1}^{K-1}+\frac{n+1}{2n+3}h_{n+1}^{K-1}\right)$$

$$\text{for } K\geq 1 \tag{16}$$

$$\frac{eE}{m}\left[\frac{n}{2n-1}\left(\frac{d}{dv}-\frac{n-1}{v}\right)g_{n-1}^0+\frac{n+1}{2n+3}\left(\frac{d}{dv}+\frac{n+2}{v}\right)g_{n+1}^0\right]+J_n g_n^0$$

$$=-v\alpha^{(0)}\left(\frac{n}{2n-1}g_{n-1}^0+\frac{n+1}{2n+3}g_{n+1}^0\right) \qquad \text{for } K=0$$

$$\frac{eE}{m}\left[\frac{n}{2n-1}\left(\frac{d}{dv}-\frac{n-1}{v}\right)g_{n-1}^K+\frac{n+1}{2n+3}\left(\frac{d}{dv}+\frac{n+2}{v}\right)g_{n+1}^K\right]+J_n g_n^K$$

$$=g_n^{K-1}-v\sum_{J=1}^{K}\alpha^{(J)}\left(\frac{n}{2n-1}g_{n-1}^{K-J}+\frac{n+1}{2n+3}g_{n+1}^{K-J}\right)$$

$$\text{for } K\geq 1 \tag{17}$$

The collision terms $J_n(v)$ in the above expressions are the same as those in a previous paper (Date et al 1990).

2.5 Computational technique

In the present calculation, the amalgamated procedure of the two-term expansion and Galerkin method which has been proposed by Yachi et al(1988) is adopted. In the method, Legendre two-term energy distributions for $n=0,1$ are calculated in the first step, then in the second step, the higher order terms for $n \geq 2$ are solved by a Galerkin method. Finally, in the third step, the first two terms are solved again with the third term which has been obtained in the second step, and a relaxation procedure from the first to third steps is repeated until the third term converges. Remarkable features of this technique are : (i) the size of the matrix solving for the coefficients of basis functions of the Galerkin method is reduced since the distribution functions $n=0,1$ have been already obtained by efficient two-term method and thus unknown functions are confined to $n \geq 2$; (ii) a set of inhomogeneous simultaneous equations, which is sloved by a Galerkin technique, is easily obtained for the higher terms ($n \geq 2$) avoiding the problem that inhomogeneous terms have zero values.

Recently Yachi et al 1991 has applied this method to FDS analysis of equation (16). However, the E/p_0 values for calculation are performed only at 1 and 100 Vcm^{-1} $Torr^{-1}$. In the present work the calculations are performed over a wide range of E/p_0 from 1 to 300 Vcm^{-1} $Torr^{-1}$ not only for FDS but also ATS experiments. Since the simultaneous equations (17) are formally analogous to (16), this amalgamated method may be applied easily to solve the equation (17). The numerical procedure and formulae used here are fundamentally the same as Yachi et al (1991).

3. Results and discussion

3.1 Collision cross sections

The collision cross sections of methane were taken from Ohmori et al (1986).

This gas has considerably large inelastic cross sections at low ($\leq$0.3eV) and high electron energies ($\geq$ 20eV). Since the two-term expansion has been reported often to fail under such condition(e.g. Pitchford et al 1981, Segur et al 1983), a multi-term technique is needed. Thus, a six-term expansion was employed in the present analysis.

3.2 Results and discussion

The drift velocities calculated for the different definitions are shown in figure 1. It is clear that W_v, W_r, V_d and W_m have the same values in an E/p_0 range from 1 to 50 Vcm^{-1} $Torr^{-1}$, and have the minimum value at $E/p_0 \simeq$ 10 Vcm^{-1} $Torr^{-1}$. Negative differential mobilities appearing below $E/p_o \simeq$ 10 Vcm^{-1} $Torr^{-1}$ may be caused by the large inelastic cross sections at low electron energies ($\leq$0.3eV) as pointed out by Ohmori et al 1986.

The difference of the drift velocities starts to increase gradually from the E/p_o at 50 Vcm^{-1} $Torr^{-1}$ as replotted on linear scales in figure 2 since ionisation occurs considerably above this E/p_0 value. Table 1 shows a comparison of the four variety of the drift velocities and other parameters (the Townsend first ionisation coefficient $\alpha_T(=\alpha^{(0)})$ and the longitudinal diffusion

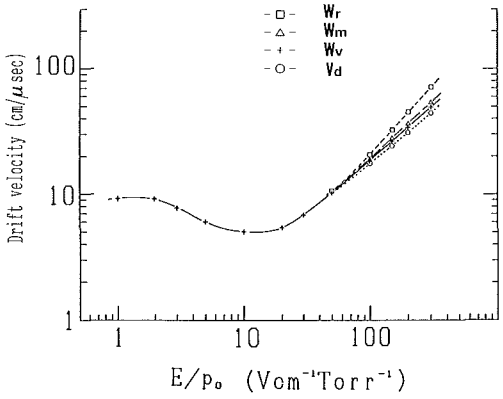

Figure 1. The electron drift velocities in methane : (W_r) the centre-of-mass drift velocity, (W_v) the mean drift velocity, (V_d) the drift velocity for the steady-state-Townsend experiment and (W_m) the mean arrival time drift velocity.

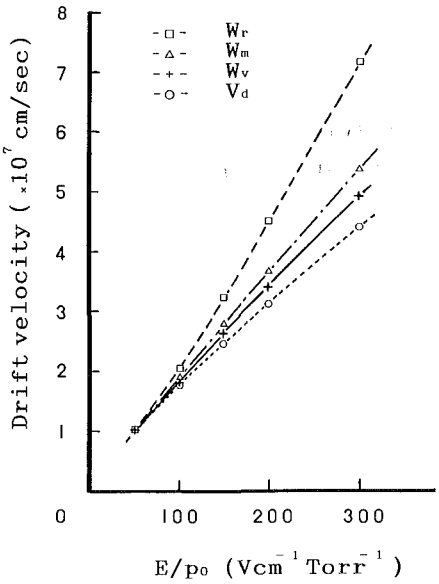

Figure 2. The electron drift velocities replotted on linear scales. The symbols for drift velocity are the same as in figure 1.

Table 1. Comparison of the drift veloties and other parameters of elcctron swarms in methane at ralatively high E/p_0 (Vcm^{-1} $Torr^{-1}$) values.

	FDS method				ATS method		
E / p_0	W_v (cm/ μs)	W_r (cm/ μs)	D_L (cm^2/ μs)	W'_m [a] (cm/ μs)	$\alpha_T(=\alpha^{(0)})$ (1 /cm)	V_d (cm/ μs)	$W_m(=1/\alpha^{(1)})$ (cm/ μs)
100	18.3	20.6	0.79	19.0	1.03	17.7	19.0
	18.4[b]	20.7[b]	0.79[b]	19.1[c]	1.03[c]	17.7[c]	19.1[c]
150	26.3	32.4	0.98	27.8	2.36	24.6	27.8
200	34.1	45.2	1.27	35.7	3.74	31.2	36.6
300	49.2	71.5	1.72	50.1	6.22	44.1	53.5

a) $W'_m = W_r - 2\alpha_T D_L$

b) Calculated by Monte carlo simulation by Yachi et al (1988).

c) Calculated by Monte carlo simulation.

coefficient D_L) at high E/p_0 values ($\geq$ 100 Vcm^{-1} Torr^{-1}). Relation between the parameters by the FDS and by the ATS methods is given as (Tagashira 1985, Kondo and Tagashira 1990) ; $W_m = W_r - 2\alpha_T D_L + 3(\alpha_T)^2\omega^{(3)} - \cdots\cdots$, where $\omega^{(3)}$ is the forth-order parameter of FDS method. To a second approximation, W'_m (which is equivalent to $W_r - 2\alpha_T D_L$) was deduced as shown in table 1. The values of W'_m are in fairly good agreement with those of W_m, although at E/p_0=300 Vcm^{-1} Torr^{-1} the discrepancy of the W_m and W'_m is about 6~7 %. It is noted that the the exact value of W_m may not be obtained by the FDS method without higher order parameters such as D_L and $\omega^{(3)}$. On the contrary the ATS analysis can deduce the values of W_m directly without calculating the higher order parameters.

The validity of the present analysis was checked by a Monte Carlo simulation at the value of E/p_0=100 Vcm^{-1} Torr^{-1} as shown in table 1. Very good agreement between the method of Boltzmann equation (FDS and ATS) and the Monte Carlo simulation was obtained.

4. Conclusion

In the present paper, the electron drift velocities defined from the flight distance spectrum, W_v and W_r, and the arrival time spectrum, V_d and W_m, in methane have been calculated over a wide range of E/p_0 from 1 to 300 Vcm^{-1} Torr^{-1}. In the calculation of the drift velocities for the FDS and ATS experiments, a multi-term method by an amalgamated procedure of the conventional two-term expansion technique and a Galerkin technique (Yachi et al 1988) was employed. The result shows that the differences of the values of the various drift velocities appear at high E/p_0 values larger than 50 Vcm^{-1} Torr^{-1}.

In particular, with focusing on the values of W_m, a comparison of the validity and accuracy of both the ATS and FDS methods was made to show that the ATS analysis is an effective means to deduce the experimental time-of-flight (TOF) parameters without resorting to higher order calculation such as to deduce the diffusion coefficient.

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