A Monte Carlo Simulation Study of Electron Drift Velocities for Conditions with Electron Impact Ionization

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A numerical calculation shows that the mean arrival time drift velocity W_m and the average velocity W_v of the electrons in isolated swarms assume very close values with common gases such as Ar, N₂, CH₄ and SiH₄. If $W_m = W_v$ is proved, there should be considerable influences on theoretical and experimental studies of electron swarms. The purpose of the present paper is to clarify if $W_m = W_v$. By a study using a Monte Carlo simulation technique and deliberately arranged model cross sections, it is found that $W_m \neq W_v$ in general. A reason why $W_m \approx W_v$ in real gases is given.

Key words : Electron drift velocity, Electron swarm, Ionization

1. Introduction

The electron drift velocity is one of the most important parameters which describe the behavior of electron swarms in gases⁽¹⁾. Until some time ago, it had been believed that the electron drift velocity assumed a value depending upon the kind of gases and the value of E/N , where E is the electric field and N is the number density of gas molecules. In previous papers⁽²⁾⁽³⁾, however, it has been shown that the electron drift velocity depends not only on the kind of gases and on the value of E/N but also on how it is defined. In the papers, it has also been shown that typical, theoretically clear-cut electron drift velocities may be defined either as the center-of-mass drift velocity W_r of the electrons in an isolated swarm, or as the simple average velocity W_v of the electrons in the swarm, or as the average velocity V_d of the electrons in the steady-state Townsend experiment.

In a companion paper to the present paper⁽⁴⁾, one of the authors (H. T.) has pointed out that a drift velocity derived from another mode of observation of isolated electron swarms is important. The drift velocity is the mean arrival time drift velocity W_m

which is defined as the ratio of the difference between two positions, in the field direction, of observation of electron swarms to the difference between the average arrival times at the positions. The importance of W_m comes from that in a most commonly used design of measurement of electron drift velocity, the mean transit time between two fixed positions in the field direction is measured and the drift velocity directly obtained from the ratio of the difference of the positions to the difference of the mean arrival times, or the transit time, is the mean arrival time drift velocity W_m .

One of the interesting problems concerning W_m is that the numerical value of W_m is found to be very close to that of W_v , the drift velocity defined as the average velocity of the electrons in an isolated swarm, for conditions even with considerable electron impact ionization. An example is shown in Table 1 for Ar⁽²⁾⁽⁵⁾. Note that when there is no ionization, nor electron attachment, W_m , W_v , W_r and V_d as well, should have the same value⁽²⁾.

In the table, the value of W_m is calculated by using two approximate formulae⁽⁴⁾ as below.

$$W_m \approx W_r - 2\alpha_T D_L \dots\dots\dots (1)$$

Table 1. Comparison of W_m and W_v (Ar).

Parameter	E/N (Td)					
	85	141	212	283	424	566
W_r (cm $\cdot\mu$ s $^{-1}$)	7.34	12.0	17.9	23.9	36.5	50.5
α_T (cm $^{-1}$)	0.231	0.669	1.29	1.92	3.16	4.30
D_L (cm $^2\cdot\mu$ s $^{-1}$)	1.01	1.06	1.14	1.24	1.49	1.87
D_3 (cm $^3\cdot\mu$ s $^{-1}$) *		0.036		0.028		0.049
W_m (cm $\cdot\mu$ s $^{-1}$) $\S$	6.87	10.58	14.96	19.14	27.1	34.48
ΔW (%) $\S$	0.15	-0.19	-0.93	-1.85	-4.24	-7.56
W_m (cm $\cdot\mu$ s $^{-1}$) $\S\S$		10.62		19.45		36.87
ΔW (%) $\S\S$		0.19		-0.26		-1.15
W_v (cm $\cdot\mu$ s $^{-1}$)	6.86	10.6	15.1	19.5	28.3	37.3

A gas number density $N=3.54\times 10^{16}$ cm $^{-3}$ is assumed.

$W_m\S = W_r - 2\alpha_T D_L$, $W_m\S\S = W_r - 2\alpha_T D_L + 3\alpha_T^2 D_3$; ΔW (%) = $100(W_m - W_v)/W_v$

The values of the parameters are taken from Ref.(2) except the values * , which are taken from Ref.(5). In this reference, the parameters are deduced from the same cross sections as in Ref.(2).

$$W_m\S\S = W_r - 2\alpha_T D_L + 3\alpha_T^2 D_3 \quad \cdots \cdots \cdots (2)$$

Here, α_T is the Townsend first ionization coefficient, D_L is the longitudinal diffusion coefficient, which is the coefficient of the second order gradient term in the field direction of the electron number density, and D_3 is the coefficient of the third order gradient term in the field direction of the electron number density, in the continuity equation of electrons for electron swarms⁽²⁾⁽⁶⁾⁽⁷⁾. The expression of W_m in Eqs (1) and (2) comes from the result of the companion paper⁽⁴⁾ in which an exact expression of W_m is obtained in an infinite series form. The expression in Eq. (1) is derived by taking the first two terms, and that in Eq. (2) by taking the first three terms, of the exact expression, and therefore the expression in Eq. (2) is expected to be more exact than that in Eq. (1) since the magnitude of each of the terms decreases very rapidly as the order of the terms increases under the conditions considered here.

In the table, some electron swarm parameters which are necessary to calculate W_m are also listed for reference.

It is seen in Table 1 that the percentage difference between the mean arrival time drift velocity W_m and the drift velocity defined as the average W_v is remarkably small even at high E/N values at which ionization is appreciable judging from the value of the ionization coefficient α_T .

The same calculation as given in Table 1 has also

been performed for N $_2$, CH $_4$ and SiH $_4$ and found that the difference between W_m and W_v are very small, only a few percent even at $E/N=566$ Td.

In all the gases, the difference between W_r , the center-of-mass drift velocity, and W_v at $E/N=566$ Td, at which ionization is considerable, differed more than 10% which may be regarded as large enough to prove the difference even with numerical calculations. Since numerical calculations are in general subject to errors due to approximation employed in theory and also due to numerical computation, it is suspected that the two drift velocities W_m and W_v are essentially the same drift velocity. Therefore, considerable efforts have been made to analytically prove that $W_m=W_v$. However, until now, it remains difficult to prove, or disprove, $W_m=W_v$.

The purpose of the present paper is to solve this problem by using a Monte Carlo simulation technique. This technique is employed here since it does not have any approximation like truncation of a series. One of the weak point of the technique is a relatively large numerical scatter in the result. However, this may be overcome firstly by using enough number of electrons to reduce the scatter to or less than a reasonable level and secondly by using fictitious cross sections with which the difference between W_m and W_v , if any, is large enough to overcome the numerical scatter.

2. Cross sections and simulation method

2.1 Collision cross sections

The main purpose of the present paper is to judge if the inductively raised hypothesis $W_m=W_v$ is generally correct. As mentioned in the previous section, the numerical examples of W_m and W_v for common gases Ar, N $_2$ and CH $_4$ and a gas, SiH $_4$, which has become very popular recently for plasma CVD applications, all strongly suggest that W_m might be equal to W_v . From a standpoint such that we prove $W_m=W_v$, we should collect as many data as possible to support $W_m=W_v$, but if we choose the opposite standpoint to disprove $W_m=W_v$, then it is a matter of trying to find at least one case against $W_m=W_v$. Taking the latter action is chosen here since it appears simpler. However, if the truth is that

q_m , q_e , q_i and q_t are respectively the momentum transfer, excitation, ionization and total cross sections. The threshold of q_e ($=9.0$ eV) is lower than that of q_i ($=10.24$ eV).

Fig. 1. Electron collision cross sections against electron energy ϵ for model gas 1.

q_m , q_e , q_i and q_t are the same as Fig. 1. The threshold of q_e ($=9.0$ eV) is higher than that of q_i ($=1.0$ eV).

Fig. 2. Electron collision cross sections against electron energy ϵ for model gas 2.

$W_m \neq W_v$, then how the examples mentioned above, with which W_m is very much likely to be equal to W_v , are explained? A possibility is that the threshold of ionization ϵ_i is located at a higher electron energy than that of excitation ϵ_e . Although a theoretical explanation is difficult, it is at least a common feature of the gases. It has been decided, therefore, to add such a set of cross sections in which $\epsilon_i < \epsilon_e$ for test. There should be no such single gases, with $\epsilon_i < \epsilon_e$, therefore such a choice of collision cross section is unreal. However, since the model and theory of electron swarms does not necessarily exclude such a case in which $\epsilon_i < \epsilon_e$ in the process of its construction and also since such a

q_m , q_e , q_i and q_t are the same as Fig. 1. The threshold of q_e ($=9.0$ eV) is higher than that of q_i ($=4.8$ eV).

Fig. 3. Electron collision cross sections against electron energy ϵ for model gas 3.

gas with $\epsilon_i < \epsilon_e$ may be "approximately created" by mixing gases, a choice of such a set of cross sections with which $\epsilon_i < \epsilon_e$ may be allowed and not too unreal.

The cross sections used in the present calculation are given in Figs 1~3. The inelastic processes, excitation and ionization here, are represented by the respective single cross sections for simplicity. The total cross section, this being the sum of the elastic and inelastic cross sections, are chosen so that the collision frequency is constant regardless of electron energy. This choice simplifies the procedure of judgement of collision in the computational routine of Monte Carlo simulation⁽⁸⁾.

The thresholds for excitation and ionization of the cross sections in Fig. 1 are chosen respectively 9.0 eV and 10.24 eV. These cross sections are shaped more or less similar to real ones when compared to those in Figs. 2 and 3.

The position and shape of the ionization cross section for Figs. 2 and 3 are chosen to be rather unreal since $\epsilon_i < \epsilon_e$ and the width of the cross section is very narrow. The ionization cross section q_i in Fig. 2 has the threshold ϵ_i at 1 eV and has a width of 3 eV, while q_i in Fig. 3 spreads from 4.8 eV to 7.8 eV. The cases for Figs. 2 and 3 may appear qualitatively similar. However, it has been deliberately arranged so that $\epsilon_i < \bar{\epsilon}$ for Fig. 2 and $\epsilon_i \approx \bar{\epsilon}$ for Fig. 3 where $\bar{\epsilon}$ is the electron mean energy.

The calculation is extended to another case in which q_i in Fig. 1 is treated in the same way as q_e so

that there is no ionization, thus making a check of the calculation since in this case all the drift velocities should assume the same value⁽²⁾.

2.2 Method of calculation

A standard Monte Carlo technique has been employed⁽⁸⁾. Briefly, the flight time τ of electrons is generated simply as follows.

$$\tau = -\nu^{-1} \ln(1 - \xi)$$

where ν is the collision frequency, taken constant in the present work, and ξ is a uniform random number between 0 and 1. During τ , the electron enjoys a free flight under the action of a uniform electric field obeying Newton's law of motion. When a collision occurs, the kind of collision is judged in such a way that the collision of a kind occurs with a probability which is proportional to the magnitude of the cross section of the kind. All the scatterings after collisions are assumed isotropic. After ionization collisions, the remaining energy of the incident electron is shared to the two electrons at a ratio of 0.2 to 0.8. All the electrons generated after ionization collisions are traced as well as the initial electrons. The electron drift velocities and other swarm parameters are sampled obeying their definitions⁽⁸⁾. To avoid the electron energy non-equilibrium effect as much as possible, the velocity distribution in equilibrium is obtained beforehand, and the initial electrons are released with the velocity distribution at a position at time $t=0$.

3. Results and discussion

The calculation is done for four cases. In case 1, the collision cross sections for model gas 1 as shown in Fig. 1 are employed and the simulation is performed at an $E/N=354$ Td.

The average velocity W_v of the electrons in an isolated swarm is sampled and shown in Fig. 4. As mentioned at the end of the previous section, the initial electrons are started with the equilibrium distribution and this is why the time required for equilibrium velocity is practically zero in Fig. 4. A reasonably accurate value may be sampled for W_v as seen from the figure.

In Fig. 5 is shown the distribution $n(z, t)$ of the arrival time of electrons at positions $z=0.2, 0.5$, and

Fig. 4. Behavior of the average electron velocity W_v of isolated swarm for case 1 (=model gas 1 at $E/N=354$ Td). The fluctuation diminishes as the number of electrons increases.

Fig. 5. Distribution of arrival time at positions in the field direction for case 1. A thousand initial electrons are injected at position $z=0$ at time $t=0$.

Fig. 6. Mean arrival time $\bar{t}$ as a function of position z for case 1 as derived from Fig. 5. Mean arrival time drift velocity W_m is obtained from the inverse of the slope of the straight line.

0.8 cm in the field direction for case 1. The mean arrival time $\bar{t}$ is calculated from the distribution and plotted in Fig. 6. The points lie well on a straight line and the mean arrival time drift velocity W_m for case 1 is obtained as the inverse of the slope of the line.

Fig. 7 shows the position of the center-of-mass of

Fig. 7. Variation of the center-of-mass $\bar{z}$ of an isolated electron swarm as a function of t for case 1. The center-of-mass drift velocity W_r is obtained as the slope of the straight line.

Fig. 8. Variation of the average electron velocity V_d for the steady-state Townsend condition for case 1. The fluctuation tends to diminish with z .

an isolated swarm $\bar{z}$ as a function of time for case 1. It is seen that the position lies practically on a straight line and from its slope the center-of-mass drift velocity is obtained. Similarly in Fig. 8 the average velocity V_d of the electrons for the steady-state Townsend condition is sampled as a function of the position.

Figs 4, 6~8 show that the present simulation can determine W_v , W_m , W_r and V_d at a reasonable accuracy.

The calculation is performed also for cases 2, 3 and 4.

In cases 2 and 3, the cross sections given in Figs 2 and 3, respectively, are used. For case 4, the calculation is performed by using the set of cross sections in Fig. 1 in which q_i , the ionization cross section, is treated also as q_e , an excitation cross section, so that there is no ionization cross section and two excitation cross sections. The E/N is assumed to be 354 Td in all the cases.

Table 2. Comparison of W_m and W_v (model gases).

	$E/N=354$ Td			
	case 1	case 2	case 3	case 4
W_r (cm $\cdot$ μ s $^{-1}$)	26.8	18.8	21.5	21.8
α_T (cm $^{-1}$)	2.7	4.2	3.2	0.0
D_L (cm 2 $\cdot$ μ s $^{-1}$)	0.95	0.73	0.69	0.83
D_3 (cm 3 $\cdot$ μ s $^{-1}$)	0.03	0.03	0.02	0.03
R_i (μ s $^{-1}$)	66.7	69.0	62.3	0.0
ϵ (eV)	6.34	6.46	6.29	6.92
W_m (cm $\cdot$ μ s $^{-1}$)	22.0	14.3	17.4	21.8
ΔW (%)	1.38	-33.80	-19.44	0.0
W_m (cm $\cdot$ μ s $^{-1}$) *	21.7	12.6	17.0	21.8
ΔW (%) *	0.0	-41.67	-21.30	0.0
W_m (cm $\cdot$ μ s $^{-1}$) **	22.1	14.2	17.7	21.8
ΔW (%) **	1.84	-34.26	-18.06	0.0
W_v (cm $\cdot$ μ s $^{-1}$)	21.7	21.6	21.6	21.8
V_d (cm $\cdot$ μ s $^{-1}$)	19.4	18.7	19.7	21.8

A gas number density $N=3.54 \times 10^{16}$ is assumed.

W_m is directly sampled by Monte Carlo simulation as other values without*.

$W_m^* = W_r - 2\alpha_T D_L$; $W_m^{**} = W_r - 2\alpha_T D_L + 3\alpha_T^2 D_3$; ΔW (%) = $100(W_m - W_v)/W_v$

The results, including those for case 1 as well, are shown in Table 2.

It is seen in the table that W_m and W_v for case 1 assume very similar values. The difference is less than 2%. From the fluctuation in simulation as seen in Figs 4~8, the difference may be judged to lie within the error of the Monte Carlo calculations. Therefore, it is difficult to say whether $W_m = W_v$ or not from the result of case 1.

If the results of simulation for case 2 are looked at, however, it is now clear that $W_m \neq W_v$. The difference ΔW amount to as large as or more than 30%. A similar result is obtained with case 3. The difference ΔW is about 20%. The differences are judged far greater than the computational error. These two cases demonstrate that $W_m \neq W_v$ in general.

Case 4 shows that $W_m = W_v = W_r = V_d$ if there is no ionization. This is a conclusion analytically drawn⁽²⁾, and this case is an indication that the present simulation is performed properly.

It is interesting to note that the electron mean energy $\bar{\epsilon}$ and ionization threshold ϵ_i are in such a relation as $\bar{\epsilon} < \epsilon_i$ in case 1. Then, ionization occurs considerably more in front of an isolated swarm

than in the rear, and this results in $W_v < W_r^{(2)}$. Note that the electron energy is higher in front than in tail of an isolated swarm since the flow of electron current due to the action of the electric field and due to diffusion add in front whereas they subtract in the rear⁽²⁾. Since $W_m < W_r$ as seen from Eq. (1) or (2), because the second and particularly third term are usually smaller than the first on the right hand side of those equations, there is certainly a possibility that $W_m \approx W_v$ in case 1. If there is an excitation cross section, the threshold of which ε_e is lower than ε_i , the electron energy is lost to excitation and the electron mean energy does not increase easily. This mechanism tends to keep $\bar{\varepsilon} < \varepsilon_i$ and so $W_v < W_r$. Therefore, what is essential is the mutual position of $\bar{\varepsilon}$ and ε_i , but $\varepsilon_e < \varepsilon_i$, as in case 1 and in real gases, assists to keep $\bar{\varepsilon} < \varepsilon_i$, which tends to give $W_v < W_r$ and when combined with $W_m < W_r$, $W_m \approx W_v$, as has been discussed.

In case 2, it is seen that $\bar{\varepsilon} > \varepsilon_i$. This leads to $W_v > W_r$ since ionization occurs more frequently in the rear than in front of an isolated swarm. The relationship between W_m and W_r is $W_m < W_r$ as seen in Eqs. (1) and (2). Therefore, $W_m < W_v$ is brought about.

The cross sections for case 3 are chosen so that the q_i assumes significant values at around $\bar{\varepsilon}$, as seen from Fig. 3 and Table 2. Namely, $\varepsilon_i \approx \bar{\varepsilon}$. This results in more or less a balanced ionization within a swarm which leads to $W_v \approx W_r$. Since $W_m < W_r$ by Eq. (1) or (2), $W_m \neq W_v$ in case 3 as well.

A check of accuracy of Eqs. (1) and (2) may be made by comparing W_m with W_m^* or W_m^{**} . It is clear that W_m^{**} calculated from Eq. (2) is in better agreement with W_m which is directly sampled in Monte Carlo simulation and therefore more accurate. This may be an indication that the formula for the accurate mean arrival time is correct.

4. Conclusions

The purpose of the present paper is to prove, or disprove, the seemingly holding relationship $W_m = W_v$, where W_m is the mean arrival time drift velocity and W_v is the average velocity of the electrons in an isolated swarm. Several examples of real gases seemed to suggest that $W_m = W_v$.

It has been shown by using a fictitious, but deliberately arranged, sets of electron-gas molecule collision cross sections that in general $W_m \neq W_v$. A reason has been given why $W_m \approx W_v$ in real gases. It has also been shown that the expression of W_m given by Eq. (2), which includes the first three terms, is more accurate than W_m given by Eq. (1) which retains the first two terms.

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