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Monte Carlo Simulation of an Electron Swarm in an Argon-like Gas

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Abstract

A Monte Carlo simulation (MCS) of an electron swarm in an argon-like gas (of atomic mass 1 a.m.u.), with Golden's cross section with a very deep minimum, is presented in order to examine the breakdown of the validity of the conventional two-term expression for the transverse diffusion coefficient D_T indicated by Milloy and Watts. It is found that the MCS value of D_T approaches the two-term value much slower than other swarm parameters such as the drift velocity W and the longitudinal diffusion coefficient D_L. The discrepancy between the MCS and two-term values of D_T revealed by Milloy and Watts is attributable to the evaluation of D_T at the long transient (correlation) stage in the MCS. It is concluded that the two-term expressions for D_T and D_L (and other swarm parameters) are sufficiently accurate even for Golden's cross section with a very deep minimum.

Because the conventional two-term solution of the Boltzmann equation is very useful for the analysis of electron swarms in gases, the validity of the two-term solution has been thoroughly examined in its various aspects. By making comparisons with electron swarm parameters obtained by the Monte Carlo simulation (MCS), Milloy and Watts (1977) indicated the breakdown of the validity of the two-term expression for the transverse diffusion coefficient D_T in an argon-like gas (of atomic mass 1 a.m.u.) with Golden's (1966) momentum-transfer cross section $\sigma_m(\epsilon)$ with a very deep minimum. It seems curious, however, that the MCS and two-term values of the drift velocity W, the mean energy $\langle\epsilon\rangle$, and even the overall energy distribution $f_0(\epsilon)$ are in agreement but D_T values disagree by up to 40% when the ratio of electric field strength to atomic number density (E/N) is about 2 Td ($\langle\epsilon\rangle \sim 1$ eV). (The longitudinal diffusion coefficient D_L was not considered.)

In this paper, a MCS of an electron swarm in the argon-like gas is presented in order to resolve this inconsistency. The Monte Carlo method is a straightforward extension of the Monte Carlo technique (Koura 1983, 1984) for the simulation of electron thermalisation in gases. At time $t = 0$, we assume that all electrons of number n_0 were isotropically released from the origin ($x = y = z = 0$) with the same energy $\langle\epsilon\rangle_0$. The scattering of electrons was taken to be isotropic and $\sigma_m(\epsilon)$ was obtained from equations (2)–(5) of Golden (1966) with $\sin(\eta_L - \eta_{L+1}) = \eta_L - \eta_{L+1}$ and $\tan\eta_L = \eta_L$ for the convenience of computation time. [This approximation has little influence on $\sigma_m(\epsilon)$ at $\epsilon < 2$ eV.] The electric field strength E was chosen as $E/N = 2$ Td so that the two-term value of $\langle\epsilon\rangle$ was about 1 eV, where the MCS

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value of D_T obtained by Milloy and Watts is considerably ($\sim 40\%$) smaller than the two-term value. The gas temperature T was chosen as 300 K, which is different from the usual condition $T = 0$ K (no thermal motion). The initial electron energy $\langle\epsilon\rangle_0$ was taken to be the two-term value (see e.g. Huxley and Crompton 1974) of 1·00 eV for $E/N = 2$ Td at $T = 300$ K in order to avoid the (long) energy relaxation. In actual calculations, time t, velocity v and position coordinates $r = (x, y, z)$ were normalised by the electron collision time $t_0 = \lambda_0/v_0$, thermal speed $v_0 = (2kT/m)^{\frac{1}{2}}$ and free path $\lambda_0 = 1/N\sigma_0$ with a unit of cross section $\sigma_0 = 1$ Å^2, respectively, where k is the Boltzmann constant and m is the electron mass; the z axis was chosen as antiparallel to the electric field E. The number of simulated electrons n_0 was taken to be 1000 for the convenience of computation time.

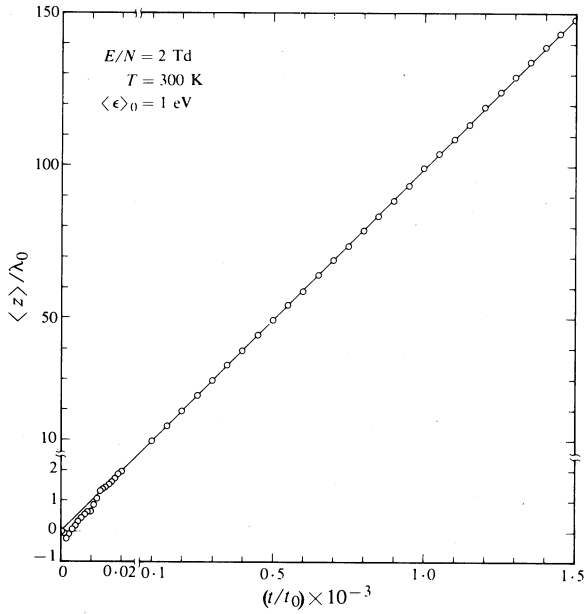

Fig. 1. Temporal behaviour of mean drift displacement $\langle z\rangle/\lambda_0$ obtained by the MCS (circles), compared with the straight line with gradient equal to the conventional two-term value of the drift velocity (W/v_0).

The MCS results indicate that the mean energy $\langle\epsilon\rangle$ maintains the initial two-term value $\langle\epsilon\rangle_0$ and the overall energy distribution $f_0(\epsilon)$ agrees with the two-term solution after ($t/t_0 \gtrsim 10$) an initial transient stage. The temporal behaviour of the mean drift displacement $\langle z\rangle/\lambda_0$ against t/t_0 is presented in Fig. 1 and compared with the straight line with gradient equal to the two-term value of the drift velocity $W/v_0 = 0{\cdot}099$. After ($t/t_0 \gtrsim 10$) an initial transient stage, the MCS gradient

$$\mathrm{d}(\langle z\rangle/\lambda_0)/\mathrm{d}(t/t_0) = W/v_0$$

agrees with the two-term value. It is noted that $\langle z\rangle/\lambda_0$ has a negative value during an initial short time ($t/t_0 \lesssim 3$) which, in fact, corresponds to the negative mobility

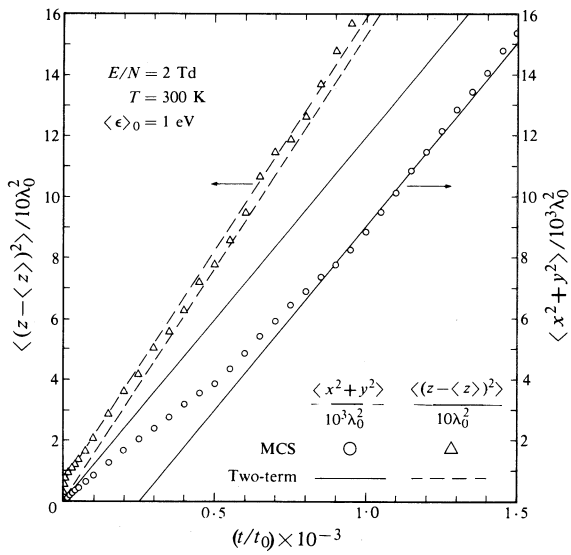

Fig. 2. Temporal behaviour of transverse, $\langle x^2+y^2\rangle/\lambda_0^2$, and longitudinal, $\langle(z-\langle z\rangle)^2\rangle/\lambda_0^2$, mean square displacements obtained by the MCS (circles and triangles), compared with the straight lines with gradients equal to the conventional two-term values of the transverse $(4D_T/v_0\lambda_0)$ and longitudinal $(2D_L/v_0\lambda_0)$ diffusion coefficients, respectively.

recently realised both theoretically (McMahon and Shizgal 1985) and experimentally (Warman *et al.* 1985). The fact that the steady-state MCS values of $\langle\epsilon\rangle$, $f_0(\epsilon)$ and W agree with the two-term values is consistent with the results of Milloy and Watts.

The temporal behaviour of the transverse, $\langle x^2+y^2\rangle/\lambda_0^2$, and longitudinal, $\langle(z-\langle z\rangle)^2\rangle/\lambda_0^2$, mean square displacements against t/t_0 is presented in Fig. 2 and compared with the straight lines with gradients equal to the two-term values of $4D_T/v_0\lambda_0 = 12{\cdot}0$ and $2D_L/v_0\lambda_0 = 0{\cdot}15$, respectively. The MCS gradient

$$\mathrm{d}\{\langle(z-\langle z\rangle)^2\rangle/\lambda_0^2\}/\mathrm{d}(t/t_0) = 2D_L/v_0\lambda_0$$

agrees with the two-term value after $(t/t_0 \gtrsim 10)$ an initial transient stage. The initial large gradient at $t/t_0 < 10$ corresponds to the transverse diffusion coefficient $(2D_T/v_0\lambda_0)$ because of the initial isotropic diffusion. It is considerably surprising that the MCS gradient

$$\mathrm{d}(\langle x^2+y^2\rangle/\lambda_0^2)/\mathrm{d}(t/t_0) = 4D_T/v_0\lambda_0$$

only agrees with the two-term value after a very long time $(t/t_0 \gtrsim 500)$. This long transient stage may be due to the fact that a long time is required for the condition

$$t \gg 1/\nu_m(\epsilon) \propto \{\epsilon^{\frac{1}{2}}\sigma_m(\epsilon)\}^{-1}$$

for the two-term solution to be valid (see e.g. Huxley and Crompton 1974). Here,

the momentum-transfer collision frequency

$$\nu_m(\epsilon) = N(2\epsilon/m)^{\frac{1}{2}}\sigma_m(\epsilon)$$

has a very small value for the electron energy ϵ at Golden's deep minimum in $\sigma_m(\epsilon)$, which dominates $D_T \propto \langle \epsilon^{\frac{1}{2}}/\sigma_m(\epsilon)\rangle$; for $\epsilon = 0{\cdot}24$ eV and $\sigma_m(\epsilon) = 0{\cdot}035$ Å^2, the condition leads to $t/t_0 \gg 10$. It is noted that the temporal behaviour of $\langle x^2+y^2\rangle/\lambda_0^2$ at the transient stage ($t/t_0 \lesssim 500$) is almost linear and, if the D_T value is evaluated at this stage, then the MCS value is about 40% smaller than the two-term value, consistent with the results of Milloy and Watts.

In the MCS of Milloy and Watts, one simulated electron was followed until the number of collisions n_c was about 10^6–10^7 and D_T was calculated from the expression

$$D_T = \lim_{\tau \to \infty} (4\tau)^{-1}\langle \{x(t+\tau)-x(t)\}^2 + \{y(t+\tau)-y(t)\}^2\rangle .$$

The time interval τ was in practice taken to be so large that there is no significant correlation between the values of $x(t+\tau)$ and $x(t)$; τ was actually taken as about $100/\langle\nu_m(\epsilon)\rangle$. In the present MCS, n_c per electron during t/t_0 is given by $n_c \sim \langle\nu_m(\epsilon)t_0\rangle(t/t_0)$. The MCS results indicate that $\langle\nu_m(\epsilon)t_0\rangle$ agrees with the two-term value of $13{\cdot}7$ at $t/t_0 \gtrsim 10$ and, therefore, n_c at $t/t_0 \lesssim 500$ is evaluated to be about 7000, which is much smaller than that of Milloy and Watts. However, the present results indicate that the correlation of D_T lasts until $t/t_0 \gtrsim 500$ and τ should be taken as $\tau/t_0 > 500$ or $\tau > 7000/\langle\nu_m(\epsilon)\rangle$, which is much larger than that of Milloy and Watts. Therefore, it is presumable that the evaluation of D_T in the MCS of Milloy and Watts corresponds to the evaluation of D_T at the long transient (correlation) stage in the present MCS.

In conclusion, the discrepancy between the MCS and two-term values of D_T revealed by Milloy and Watts is attributable to the evaluation of D_T at the long transient (correlation) stage in the MCS and the two-term expressions for D_T and D_L (and other swarm parameters) are sufficiently accurate even for Golden's cross section with a very deep minimum.

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