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Computer calculation of positron drift velocities in He, Ne and Ar

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Abstract. The drift velocities of positrons in rare gases, He, Ne and Ar have been calculated at various temperatures. The drift velocity depends quite sensitively on the strength of the electric field and temperature.

Keywords. Positron drift velocities; rare gases.

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1. Introduction

The drift motion of a positron swarm in a gas assembly, under the influence of external fields, is determined by positron-atom interaction processes, like scattering, annihilation etc. For slow positrons, energy less than the positronium formation threshold, E_{th} (E_{th} = 9, 14·7, 17·7 eV for argon, neon and helium respectively), elastic scattering is dominant. Positrons also undergo annihilation with outermost electrons of atoms. They have a finite lifetime which can be measured experimentally (Canter 1972; Griffith 1978). The lifetime can be influenced by external fields like electric field, magnetic field and temperature of the gas assembly (Grover 1977, 1982). This parameter has been used to test positron-atom scattering and annihilation models. There can be other parameters such as drift velocity, average energy, diffusion coefficient, etc which may be of physical interest in the investigation of the behaviour of positrons in gases and gas-mixtures. Their theoretical study and experimental determination can also shed further light on the positron-atom interaction model.

The effect of external fields on positron lifetime and average energy has been recently investigated (Grover 1982). However, there does not appear to be any systematic theoretical study of positron drift in rare gases and the influence of temperature on this. We have done this by performing computer calculations and simulating positron distributions. From this analysis, drift velocities in three gases, helium, neon and argon have been obtained over the temperature range 150–3000 K. The drift velocity depends on temperature and electric field quite appreciably.

2. Method of study

We consider positrons with energy less than the positronium formation threshold, E_{th}. In this energy region, only elastic scattering and annihilation processes are dominant. For a free positron moving in a homogeneous gas assembly, it can be assumed that its behaviour is described adequately in terms of single atom interaction model. If $N(0)$ is

the initial number of positrons emitted by a source in the gas assembly and $N(t)$ is the number of positrons remaining at time t, then the annihilation time dependent spectrum is given by

$$\frac{1}{N(0)}\frac{\mathrm{d}N(t)}{\mathrm{d}t} = -\int \nu_a(v) f(\mathbf{v}, t)\,\mathrm{d}\mathbf{v}. \tag{1}$$

Here $f(\mathbf{v}, t)$ is the positron time-dependent velocity distribution function. $\nu_a(v)$ is the velocity dependent positrons annihilation rate and $v = |\mathbf{v}|$ is the velocity of positrons. If $\sigma_a(v)$ is the annihilation cross-section, then $\nu_a(v) = nv\sigma_a(v)$, n is the density of gas. When an electric field, E, is applied to the (positron + gas atoms) assembly, the distribution function can be obtained by solving the Boltzmann equation (Huxley and Crompton 1974):

$$\frac{\partial f(\mathbf{v}, t)}{\partial t} + \frac{e\mathbf{E}}{m}\cdot\frac{\mathrm{d}f(\mathbf{v}, t)}{\mathrm{d}\mathbf{v}} = \left[\frac{\delta f}{\delta t}\right]_{\text{coll}} \tag{2}$$

Here e and m are the positron charge and mass respectively. $[\delta f/\delta t]_{\text{coll}}$ is the collision term which consists of two parts: one due to elastic scattering and the other due to annihilation.

The distribution function may be expanded in the velocity space as:

$$f(\mathbf{v}, t) = f_0(v, t) + \frac{\mathbf{v}}{v}\cdot\mathbf{f}_1(v, t) \tag{3}$$

retaining only the first two terms. $f_0(v, t)$ indicates the spherically symmetric part and f_1 denotes the asymmetry present in the distribution function. In the expansion of (3), it is assumed that $|\mathbf{f}_1| \ll f_0$. Use of (3) in (2) leads to the following equations for f_0 and f_1 (Huxley and Crompton 1974):

$$\frac{\partial \mathbf{f}_1}{\partial t} + \frac{e\mathbf{E}}{m}\frac{\partial f_0}{\partial v} = \left[\frac{\delta \mathbf{f}_1}{\delta t}\right]_{\text{coll}} = \left[\frac{\delta \mathbf{f}_1}{\delta t}\right]_m + \left[\frac{\delta \mathbf{f}_1}{\delta t}\right]_a, \tag{4}$$

$$\frac{\partial f_0}{\partial t} + \frac{e}{3mv^2}\frac{\partial}{\partial v}[v^2\mathbf{E}\cdot\mathbf{f}_1] = \left[\frac{\delta f_0}{\delta t}\right]_{\text{coll}} = \left[\frac{\delta f_0}{\delta t}\right]_m + \left[\frac{\delta f_0}{\delta t}\right]_a, \tag{5}$$

where the collision term has been split into scattering and annihilation terms denoted by the subscripts m and a respectively.

Equations (4) and (5) are coupled equations. These equations are to be solved to obtain the positron distribution function.

Following Holestein (1946), we approximate the collision terms of (4) as:

$$\left[\frac{\delta \mathbf{f}_1}{\delta t}\right]_m = -\nu_m(v)\,\mathbf{f}_1 \text{ and } \left[\frac{\delta \mathbf{f}_1}{\delta t}\right]_a = -\nu_a(v)\mathbf{f}_1, \tag{6}$$

where ν_m is the positron-atom scattering rate. If $\sigma_m(v)$ is the scattering cross-section, then $\nu_m(v) = nv\,\sigma_m(v)$. At times much greater than the slowing down time of positrons, the time dependence of f_1 can be ignored and that of f_0 approximated by $-\lambda f_0$ where λ is the decay rate, inverse of positron lifetime. Thus, from (4) and (5):

$$\mathbf{f}_1 = -\frac{e\mathbf{E}}{m(\nu_a + \nu_m)}\frac{\mathrm{d}f_0}{\mathrm{d}v} \tag{7}$$

$$-\lambda f_0(v)+\frac{e}{3mv^2}\frac{\mathrm{d}}{\mathrm{d}v}(v^2\mathbf{E}\cdot\mathbf{f}_1)=\left[\frac{\delta f_0}{\delta t}\right]_m+\left[\frac{\delta f_0}{\delta t}\right]_a. \tag{8}$$

The scattering collision term of (8) for elastic scattering of positrons from atoms can be calculated (Huxley and Crompton 1974) and is given as:

$$\left[\frac{\delta f_0}{\delta t}\right]_m=\frac{m}{M}\frac{1}{v^2}\frac{\mathrm{d}}{\mathrm{d}v}\left[v^2\nu_m\left(f_0+\frac{kT}{mv}\frac{\mathrm{d}f_0}{\mathrm{d}v}\right)\right]. \tag{9}$$

While the annihilation term can be written as:

$$[\delta f_0/\delta t]_a=-\nu_a(v)f_0(v). \tag{10}$$

Here, M is the mass of the gas atom, T is the temperature of the assembly and k is the Boltzmann constant. Use of (7), (9) and (10) in (8) gives after an integration over velocity:

$$\left[\frac{a^2v^2}{3(\nu_a+\nu_m)}+\frac{kT\nu_m v^2}{M}\right]\frac{\mathrm{d}f_0}{\mathrm{d}v}+\mu\nu_m v^3 f_0(v),$$
$$=\int_0^v(\nu_a-\lambda)v'^2 f_0(v')\,\mathrm{d}v' \tag{11}$$

where $a=eE/m$ is the positron acceleration and $\mu=m/M$. Equation (11) determines the isotropic part of the distribution function, while the anisotropic part can be obtained from (7). Further $f_0(v)$ is normalized according to $4\pi\int_0^\infty v^2 f_0(v)\,\mathrm{d}v=1$ and satisfies the conditions $f_0(v=0)=$ finite and $f_0(v=\infty)=0$. The total positron density, at times when equilibrium has been reached, can be obtained from

$$n_p=4\pi\int_0^\infty v^2 f_0(v)\,\mathrm{d}v. \tag{12}$$

The drift velocity, $\mathbf{W}$, due to an electric force $e\mathbf{E}$, is given by (Huxley and Crompton 1974)

$$\mathbf{W}=-\frac{4\pi}{3n_p}\int_0^\infty v^3\,\mathbf{f}_1(v)\,\mathrm{d}v. \tag{13}$$

Substituting for f_1 from (7) in (13)

$$V_d=|\mathbf{W}|=\left(\frac{4\pi}{3}\right)\left(\frac{e|\mathbf{E}|}{mn_p}\right)\int_0^\infty\frac{v^3}{(\nu_a+\nu_m)}\frac{\mathrm{d}f_0}{\mathrm{d}v}\,\mathrm{d}v \tag{14}$$

In most systems, $\nu_m\gg\nu_a$. It is quite reasonable to take $(\nu_a+\nu_m)\cong\nu_m$. The effect of annihilation on drift velocity enters *via* the distribution function.

The drift velocity can be obtained from (14), if the distribution function derivative is known. This can be calculated numerically by solving (11). An efficient numerical algorithm to solve this equation for realistic scattering and annihilation rates has been described earlier (Grover 1977). This yields the distribution function and its derivative as well. Substitution of $\mathrm{d}f_0/\mathrm{d}v$ in (14) yields the positron drift velocity as a function of external electric field and temperature of gas.

To perform the computations, and simulate the distribution functions and its derivatives, we need data on the scattering and annihilation cross-sections. Several workers (Ghosh *et al* 1982) have studied scattering of positrons from gases and

investigated their cross-sections. But the data used in the present work are as follows: Companeau and Humberston (1977) model H_5 for helium, McEachran *et al* (1978) for neon and Grover (1979) for argon. These have been chosen because they give reasonable agreement of positron lifetimes in these gases with experiment.

3. Results and discussion

The drift velocities have been obtained at various temperatures as a function of external electric field. The temperature range considered is 150–3000 K for all the gases. The results for the three gases are as:

3.1 *Helium*

Figure 1 shows the dependence of drift velocity on electric field. The field is varied over the range 0–30 V cm^{-1} amagat^{-1}. It is seen that the drift velocity is zero at $E = 0$ (as it should be) and then increases with electric field. It goes through a maximum and then starts decreasing. The maximum occurs at $E \simeq 1$ V cm^{-1} amagat^{-1} for higher temperatures, but shifts to $E \simeq 2$ V cm^{-1} amagat^{-1} for temperatures around 500 K and lower. For $E \gtrsim 10$ V cm^{-1} amagat^{-1}, V_d decreases slowly. This behaviour is present at all temperatures. The rapid variations in drift velocity at lower fields are due to the fact that velocity of positrons is such (at these fields) that the scattering and annihilation cross-sections undergo sharp variations. At higher velocities, variations are not as fast. So, as the electric field strength is raised, velocity of positrons increases and hence the sharp variations in drift velocity also diminish. The annihilation decay

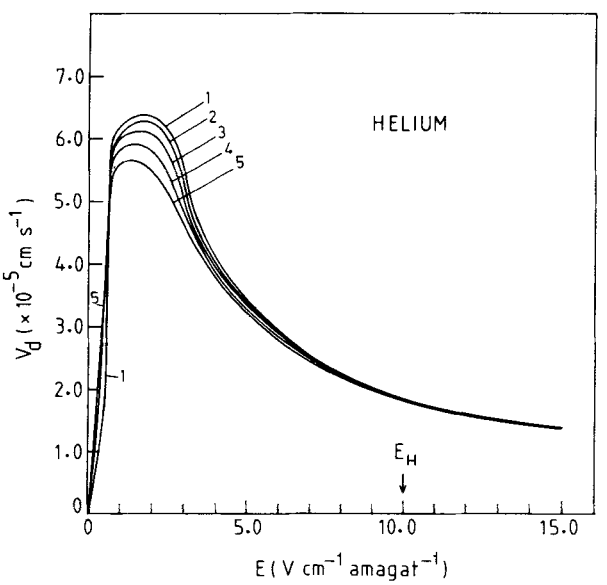

Figure 1. Variation of drift velocity, V_d, with electric field in helium gas. Curves 1–5 are for temperatures, T = 150, 500, 1000, 2000 and 3000 K. E_H indicates the field beyond which V_d tends to be almost independent of temperature of gas.

rate of positrons in helium also exhibits sharp drop at low fields (Grover 1979). Values of drift velocity at $T = 300\,K$ as a function of electric field are presented in table 1.

3.2 *Neon*

The dependence of drift velocity on electric field over the range 0–30 $V\,cm^{-1}$ in neon gas is shown in figure 2. The results of V_d for $T = 300\,K$ are given in table 1. The drift

Table 1. Positron drift velocities ($\times 10^5\,cm^{-1}$) at room temperature (300 K) in helium and neon.

E ($V\,cm^{-1}$ amagat^{-1})	V_d	
	Helium	Neon
0·1	0·354	0·251
0·2	0·685	0·680
0·5	1·69	1·87
1	5·95	2·26
2	6·31	2·59
3	4·99	2·78
5	3·33	3·03
10	1·88	2·38
20	1·20	1·39
30	1·09	0·99

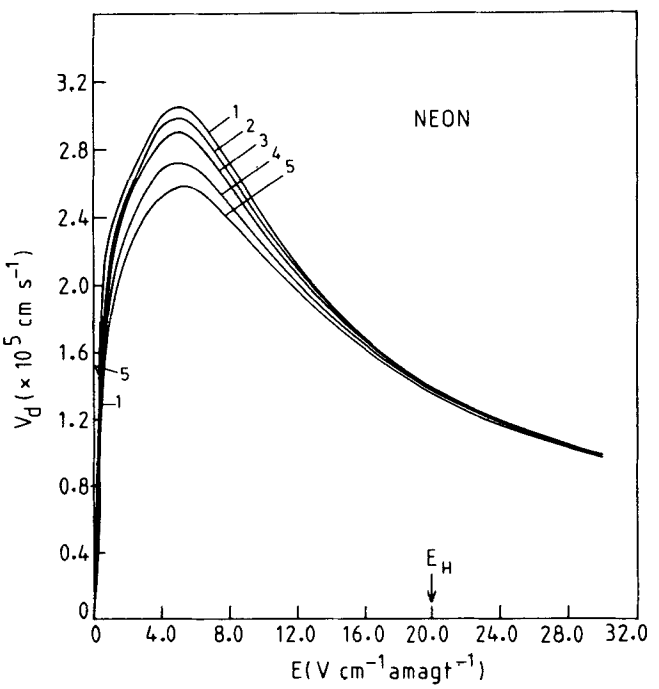

Figure 2. Positron drift velocity, V_d, *vs* electric field E in neon. Curves 1–5 are for the same temperature values as indicated in figure 1. E_H has the same significance as in figure 1.

velocity increases with electric field, goes to a maximum value and starts decreasing. The maximum value of drift velocity is reached for $E \simeq 5\,\mathrm{V\,cm^{-1}}$ amagat^{-1}. At higher field ($\lesssim 20\,\mathrm{V\,cm^{-1}}$) the dependence of drift velocity on temperature is reduced. The field dependence of drift velocity on electric field is similar to that in helium except that the maxima are now shifted to higher fields and are broader.

3.3 *Argon*

Figure 3 presents the dependence of drift velocity on electric field in argon for the temperature range 150–3000 K. The field has been varied over the range 0–150 $\mathrm{V\,cm^{-1}}$ amagat^{-1}. The drift velocity increases continuously with electric field, goes through a maxima and then decreases. At lower fields and temperatures, V_d increases almost linearly. The slope of curve 1 ($T = 150$ K) is $4 \times 10^3\,\mathrm{cm^2\,sec^{-1}\,V^{-1}}$ for the field range 0–20 $\mathrm{V\,cm^{-1}}$ amagat^{-1} which increases with temperature. Its value is $6{\cdot}1 \times 10^4$ $\mathrm{cm^2\,sec^{-1}\,V^{-1}}$ at $T = 3000$ K. As compared to helium and neon, increases in V_d in argon are not very sharp. This is because the scattering and annihilation cross-sections of argon do not exhibit sharp variations as the cross-sections of helium and neon do. However, drift velocity maxima are broader in argon and they shift with temperature. Lower temperature maxima occur at higher fields. Crossing of the curves takes place near maxima at fields $\approx$ 45–50 $\mathrm{V\,cm^{-1}}$.

Numerical values of drift velocity at $T = 300$ K at various fields are presented in table 2.

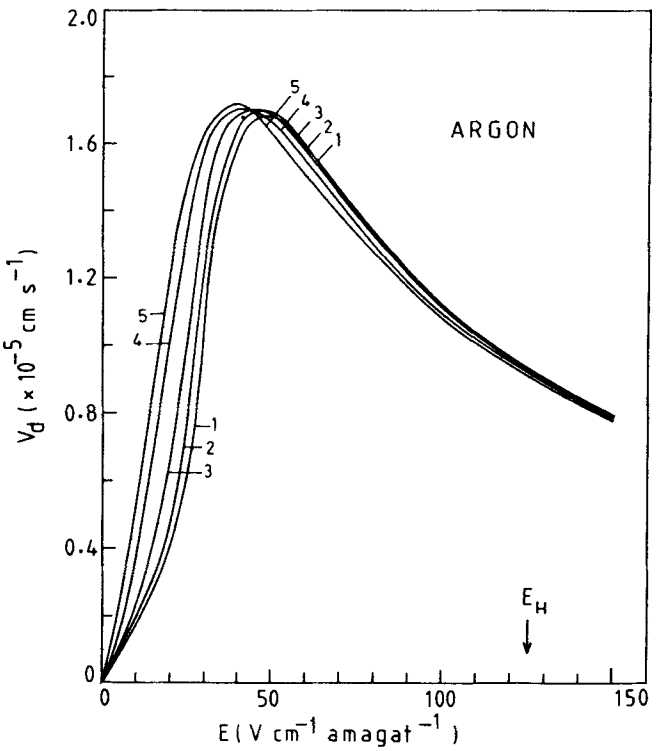

Figure 3. Electric field dependence of positron drift velocity in argon. Curves 1–5 are for the temperature values indicated in figure 1. E_H has the same meaning as in figure 1.

Table 2. V_d ($\times 10^5$ cm^{-1}) in argon at T = 300 K.

E (V m^{-1} amagat^{-1})	V_d (argon)
1	0·019
3	0·058
5	0·096
10	0·19
20	0·39
50	1·69
100	1·12
150	0·79

We find from figures 1–3 that drift velocity depends on the fields in a rather complicated way. This is because it is determined by the nature of dependence of elastic momentum transfer and annihilation cross-sections on positron velocity which by itself is not simple. However, the present computer calculations enable us to derive the following broad conclusions.

At low fields, drift velocity increases with electric field. It also increases with increase of temperature of gas at a given field, less than a certain value, E_x ($E_x \approx 0{\cdot}6$ V cm^{-1} for helium, $\approx 0{\cdot}5$ V cm^{-1} for neon and ≈ 45 V cm^{-1} for argon). This appears to be because at these electric/temperature fields, energy of positrons is such that elastic and annihilation cross-sections decrease strongly with velocity. Elastic scattering tends to make the distribution function isotropic and hence decrease the drift velocity (Engel 1965). When elastic cross-section decreases, the distribution function becomes more anisotropic. This leads to increase in the drift velocity. Large annihilation cross-section introduces more anisotropy in the distribution function and hence V_d is more. But when annihilation cross-section decreases anisotropy is reduced and so is the drift velocity of positrons. The increase in drift velocity for the fields $\lesssim E_x$ is due to the fact that increase in V_d due to decrease in elastic cross-section is more than the reduction in V_d due to lowering of annihilation cross-section.

The drift velocity passes through a maxima for certain electric fields, E_{max}. Value of $E_{max} \approx$ 1-2 V cm^{-1} for helium, ≈ 5 V cm^{-1} for neon and $\approx$ 40–50 V cm^{-1} for argon. Around such fields, the distribution function is more anisotropic and hence the drift velocity is large.

We notice further that for higher field strengths, $E > E_{max}$, drift velocity decreases with electric field. Moreover, at field strengths E_H ($E_H \approx 10$ V cm^{-1} for helium, ≈ 20 V cm^{-1} for neon and ≈ 125 V cm^{-1} for argon), V_d tends to be almost independent of the gas temperature. This can be explained keeping in view that at high fields, the temperature term in (11) is much less than the electric field term (first term in square bracket of this equation). Ignoring annihilation, we get from (11):

$$\frac{df_0}{dv} \simeq -\frac{3\mu v v_m^2}{a^2} f_0 \tag{15}$$

and the drift velocity from (14) becomes:

Table 3. Positron annihilation decay rates in various gases at T = 3000 K and zero electric field.

Gas	Z_{eff}	
	Theory	Expt.
He	3·85 (Campeanu and Humberston 1977; Grover *et al* 1980)	3·94 ± 0·02 (Grover *et al* 1980; Coleman *et al* 1975)
Ne	6·99 (Grover: Unpublished)	5·99 ± 0·08 (Coleman *et al* 1975)
Ar	27·31 (Grover 1979)	26·77 ± 0·09 (Coleman *et al* 1975)

$$V_d \simeq \left(\frac{4\pi\mu}{n_p}\right)\left(\frac{m}{eE}\right)\int_0^\infty \nu_m v^4 f_0 \, dv. \tag{16}$$

Thus, the drift velocity should decrease with increase in electric field and be almost independent of the gas temperature. The small dependence, observed in the curves, is because the distribution function depends on the temperature and the annihilation, which has been ignored in the present argument.

The type of variations observed in the three gases are related to the velocity dependence of annihilation and scattering rates. These are e^+-atom interaction model-dependent. If we were to use some other model, the numerical value and the variation of drift velocity may be different, but the overall features could be similar. Thus experimental study of variation of e^+ drift velocity in gases can provide an additional parameter to examine the validity of the e^+-atom interaction model employed. Moreover, the drift velocity may prove to be a more sensitive parameter to the details of e^+-atom interaction model, as it is determined by the velocity gradient of distribution function, equation (14).

At present, there does not appear to be any reported measurements of drift velocity in helium, neon, argon, krypton and xenon, though some measurements in hydrogen gas (Bose *et al* 1981) exist. However to check our computations and simulated results, we obtained the annihilation decay rates, $\bar{Z}_{eff} = \lambda/\pi r_0^2 cn$ (r_0 = classical electron radius, c = velocity of light), for the three gases at $T = 300$ K and zero electric fields and compared with experiments (Grover *et al* 1980; Coleman *et al* 1975). The results are presented in table 3. We observe that the agreement is reasonable except in neon.

The present computer-based results suggest that it will be interesting to look into drift velocity measurements experimentally in rare gases and explore the effects of various fields on this parameter.

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