

Numerical Simulation of Positron Diffusion in the Heavy Noble Gases Ar, Kr and Xe

Vikram Singh^A and P. S. Grover^B

^A Department of Physics and Astrophysics,
University of Delhi, Delhi 110 007, India.

^B Department of Computer Science,
University of Delhi, Delhi 110 007, India.

Abstract

Numerical simulation has been carried out of positron annihilation and diffusion under the influence of an external temperature and electric field in heavy noble gases. The electric field was varied over the range 0–200 V cm⁻¹ amagat⁻¹ (1 amagat $\equiv 2.687 \times 10^{19}$ atoms cm⁻³), whereas the temperature was varied from 300 to 3000 K. It is observed that the decay constant \bar{Z}_{eff} increases with increasing atomic mass of the interacting gases He, Ne, Ar, Kr and Xe, while the diffusion coefficient decreases except in the case of neon.

1. Introduction

The behaviour of slow positrons in monoatomic gas assemblies has been the subject of investigation by many workers in recent years. Such studies, apart from providing a test of proposed positron-atom interaction models, also give an insight into other characteristics of positrons, such as slowing down, positronium formation, diffusion, drift and lifetime etc. At energies below the positronium formation threshold (8.96 eV for Ar, 7.20 eV for Kr and 5.33 eV for Xe), elastic scattering and annihilation processes play a dominant role in determining the behaviour of positrons. The positrons undergo annihilation with the outermost atomic electrons and, thus, have a finite lifetime. This has been studied experimentally by Lee *et al.* (1969), Orth and Jones (1969), Canter (1972), Lee and Jones (1974) and Coleman *et al.* (1975) for Ar, and by Griffith (1979), Heyland *et al.* (1982) and Charlton (1985) for Kr and Xe.

Theoretical studies of the lifetime of positrons have been carried out by Schrader and Svetic (1982) and Campeanu (1982) for Kr and Xe. The influence of external fields on the positron annihilation decay constant λ in Ar has been studied by Grover (1977, 1980). The results by various authors for Ar, Kr and Xe are summarised in Table 1.

Recently, there have been more elaborate and accurate cross-section calculations for He, Ne, Ar, Kr and Xe based on the polarised orbital approximation by McEachran and Stauffer (1977) and McEachran *et al.* (1978, 1979, 1980). Using this model, diffusion and drift characteristics have been studied by Sinha and Grover (1985) in the light gases He and Ne, but not for the heavy noble gases Ar, Kr and Xe. The effects of external temperature and electric fields have also not been studied. Therefore, it is of interest to investigate the findings of positron behaviour in heavy gases based on the McEachran model.

Table 1. Annihilation decay constant \bar{Z}_{eff} at $T = 300 \text{ K}$ and $E = 0$

	Ar	Kr	Xe
Experimental results	$27.3 \pm 1.3^{\text{A}}$	$65.7 \pm 0.3^{\text{D}}$	$320 \pm 5^{\text{D}}$
	$26.77 \pm 0.09^{\text{B}}$	66.8^{E}	$320 \pm 1^{\text{E}}$
	$26.60 \pm 0.51^{\text{C}}$		
Theoretical values	27.311^{F}	$57.6 \pm 2.9^{\text{G}}$	$217 \pm 11^{\text{G}}$
		57.11^{H}	158.36^{H}
	30.131^{I}	55.9^{I}	161.23^{I}

^A Orth and Jones (1969). ^B Coleman *et al.* (1975). ^C Lee and Jones (1974).
^D Heyland *et al.* (1982). ^E Griffith (1979). ^F Grover (1980). ^G Schrader
and Svetic (1982). ^H Campeanu (1982). ^I Present work.

2. Method of Computation

The behaviour of positrons, at energies below the positronium formation threshold and interacting with a homogeneous gas assembly at temperature T , under the influence of a steady electric field E , is governed by the Boltzmann diffusion equation (Grover 1977)

$$\left(\frac{e^2 E^2}{3m^2 v_m^2(v)} + \frac{kT}{M} \right) v \frac{\partial f(v)}{\partial v} + \frac{m}{M} v^2 f(v) = \frac{1}{v_m(v) v} \int_0^v \{ \nu_a(v') - \lambda \} v'^2 f(v') dv', \quad (1)$$

where e , m , v and $f(v)$ are the positron charge, mass, velocity and velocity distribution function respectively, M is the mass of the gas atom, k is Boltzmann's constant and $\nu_a(v)$ and $\nu_m(v)$ are the velocity dependent positron annihilation and scattering rates respectively, defined by

$$\nu_a(v) = nv \sigma_a(v), \quad \nu_m(v) = nv \sigma_m(v),$$

where n is the gas density and $\sigma_a(v)$ and $\sigma_m(v)$ are the positron annihilation and scattering cross sections respectively. The annihilation decay constant λ is given by (Grover 1977)

$$\lambda(E, T) = \int_0^\infty \nu_a(v) v^2 f(v) dv / \int_0^\infty v^2 f(v) dv. \quad (2)$$

The diffusion coefficient D of the positron swarm can be obtained from (Huxley and Crompton 1974)

$$D(E, T) = \frac{4\pi}{3n_p} \int_0^\infty \frac{v^4}{\nu_a(v) + \nu_m(v)} f(v) dv, \quad (3)$$

where the positron density is

$$n_p = 4\pi \int_0^\infty v^2 f(v) dv.$$

In most systems $\nu_m \gg \nu_a$, and therefore it is quite reasonable to take

$$\nu_a(v) + \nu_m(v) \approx \nu_m(v).$$

We see that the above parameters can be obtained provided the positron velocity distribution function is known, and this can be obtained by solving equation (1). To do this it is essential that $\sigma_a(v)$ and $\sigma_m(v)$ are known. The data for $\sigma_a(v)$ and $\sigma_m(v)$ in Ar, Kr and Xe needed in our computations have been taken from McEachran *et al.* (1979, 1980). The cross sections have a complicated dependence on velocity and, as such, the Boltzmann equation cannot be solved analytically. Therefore, we have solved it numerically and obtained the distribution function by performing extensive computer calculations. The density of gas assemblies has been taken to be 1 amagat, the temperature range considered was 300 to 3000 K, while the electric field has been varied over the range 0–200 V cm⁻¹ amagat⁻¹.

3. Results and Discussion

The results of our calculations are presented in Figs 1–5 in a form which facilitates a comparative study of various gas systems. Fig. 1 shows the dependence obtained of the decay constant on the temperature. Here we have redefined the decay constant as $\bar{Z}_{\text{eff}} = \lambda/\pi r_0^2 c n$, where $r_0 = e^2/mc^2$ is the classical electron radius, c the velocity of light and n the gas density. The decay constant decreases with an increase in temperature of the gas assembly. The variation of \bar{Z}_{eff} with temperature for the lighter gases He and Ne calculated by Sinha and Grover (1985) are also shown for comparison (and similarly in Figs 2–5). We find that the dependence of \bar{Z}_{eff} on temperature is very small in He [$\bar{Z}_{\text{eff}}(300) = 4.013$ and $\bar{Z}_{\text{eff}}(3000) = 3.764$] and Ne [$\bar{Z}_{\text{eff}}(300) = 6.989$ and $\bar{Z}_{\text{eff}}(3000) = 6.333$], the relative decrease being 6.20% for He and 8.38% for Ne. The decay constant exhibits greater variation with temperature for the heavy gases for temperatures ≤ 1000 K for Ar, ≤ 2000 K for Kr and ≤ 2500 K for Xe. At higher temperatures, the variation is fairly small. The relative decrease over the range 300–3000 K is 41.19% for Ar, 59.12% for Kr and 79.39% for Xe. Thus, we find that the temperature dependence becomes more pronounced with increasing atomic mass.

Fig. 2 shows the variation of \bar{Z}_{eff} with electric field at the room temperature of 300 K. We observe that the variation is quite marked for fields up to about 5 V cm⁻¹ amagat⁻¹ for He and Ne, but for the heavier gases the range over which large variations are observed increases: ≈ 40 V cm⁻¹ amagat⁻¹ for Ar, ≈ 50 V cm⁻¹ amagat⁻¹ for Kr and ≈ 70 V cm⁻¹ amagat⁻¹ for Xe. For stronger fields \bar{Z}_{eff} becomes almost constant. It is interesting to note that these ranges increase with atomic mass.

The variation of \bar{Z}_{eff} with atomic mass of the gas at a temperature of 300 K and zero electric field is shown in Fig. 3. The decay constant is found to be an increasing function of the atomic mass of the interacting gas.

Fig. 4 depicts the variation of the diffusion coefficient with temperature for a zero electric field. For each noble gas, the diffusion coefficient decreases with an increase in atomic mass, except for Ne. The positron diffusion coefficient in Ne is more than in He, unlike the positron annihilation rate, due to the fact that the momentum transfer rate in Ne is less than that in He beyond the positron energy of 0.076 eV.

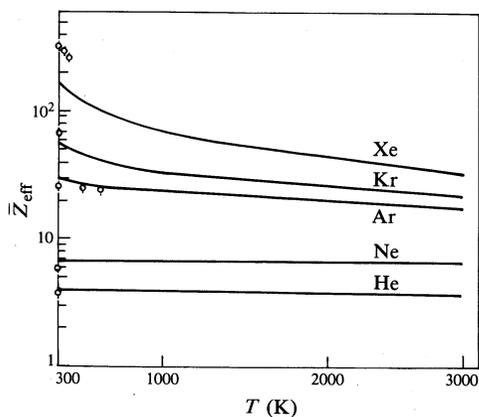


Fig. 1. Variation of the annihilation decay constant with temperature at zero electric field. Circles show the experimental values by Lee and Jones (1974) for Ar, by Lee *et al.* (1969) for He, Ne and Ar and by Heyland *et al.* (1982) for Kr and Xe.

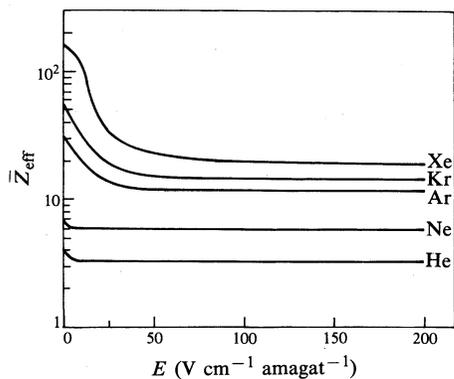


Fig. 2. Dependence of the annihilation decay constant on the electric field at a temperature of 300 K.

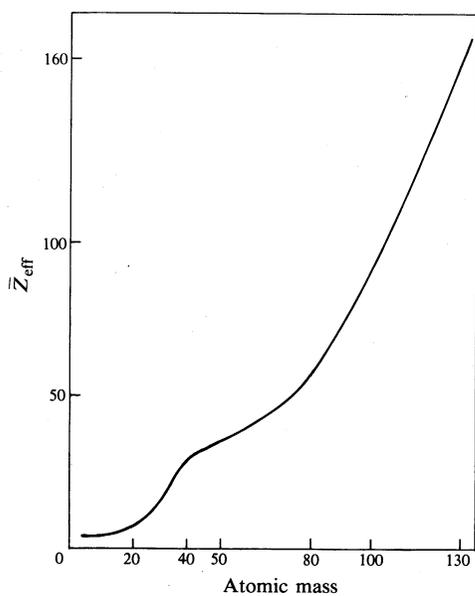


Fig. 3. Variation of Z_{eff} with atomic mass of the noble gases.

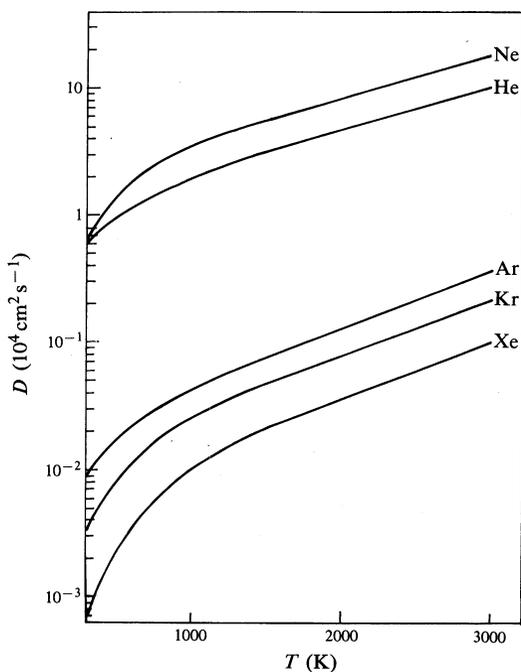


Fig. 4. Effect of temperature on the diffusion coefficient at zero electric field.

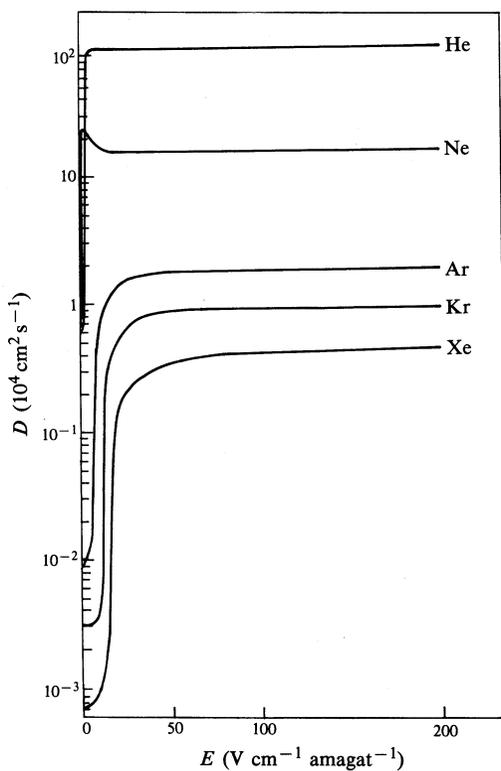


Fig. 5. Variation of the diffusion coefficient with electric field at a temperature of 300 K.

The dependence of the diffusion coefficient on the electric field is presented in Fig. 5. We find that the diffusion coefficient increases sharply with electric field at low field strengths ($\lesssim 7 \text{ V cm}^{-1} \text{ amagat}^{-1}$ for He and Ne, $\lesssim 50 \text{ V cm}^{-1} \text{ amagat}^{-1}$ for Ar, $\lesssim 60 \text{ V cm}^{-1} \text{ amagat}^{-1}$ for Kr and $\lesssim 80 \text{ V cm}^{-1} \text{ amagat}^{-1}$ for Xe) and then becomes almost constant for stronger fields. In the case of Ne, there is a jump at $E \approx 0.7 \text{ V cm}^{-1} \text{ amagat}^{-1}$ in the value of the diffusion coefficient, which appears to be the result of a fairly deep Ramsauer minimum in the momentum transfer rate at low energies (see Table 2).

Table 2. Ramsauer minima for the five noble gases

Gas	σ_m^A	Energy (eV)
He	0.0293	1.963
Ne	0.0527	0.127
Ar	1.450	1.437
Kr	3.170	1.410
Xe	(Ramsauer minimum not indicated)	

^A McEachran and Stauffer (1977) and McEachran *et al.* (1978, 1979, 1980). Units of σ_m are πa_0^2 , where a_0 is the Bohr radius.

We observe that the diffusion coefficient shows more variation with the electric field than the annihilation constant. This is because the annihilation constant depends predominantly on ν_a , while the diffusion coefficient depends largely on ν_m . Moreover, the momentum transfer cross sections depend more sensitively on energy than the annihilation cross sections. Values of the diffusion coefficient at room temperature are $6929, 6966, 41.69, 30.81$ and $7.476 \text{ cm}^2 \text{ s}^{-1}$ for He, Ne, Ar, Kr and Xe respectively.

4. Conclusions

As shown in Table 1, the agreement between experiment and our calculated result for the annihilation rate is reasonable for Ar and Kr, but not for Xe where the discrepancy is very large. We are not able to compare our calculated diffusion coefficients with experimental data because no measurements have so far been made. The present results are expected to provide impetus for such measurements. An experimental determination of the diffusion coefficient and annihilation decay constant can help us to examine the accuracy of the approach used to estimate ν_a and ν_m for noble gases.

References

- Campeanu, R. I. (1982). *Can. J. Phys.* **60**, 615.
 Canter, K. F. (1972). *Contemp. Phys.* **13**, 45.
 Charlton, M. (1985). *Rep. Prog. Phys.* **48**, 737.
 Coleman, P. G., Griffith, T. C., Heyland, G. R., and Killeen, T. L. (1975). *J. Phys. B* **8**, 1734.
 Griffith, T. C. (1979). *Adv. At. Mol. Phys.* **15**, 1035.
 Grover, P. S. (1977). *J. Phys. B* **10**, 2269.
 Grover, P. S. (1980). *Z. Naturforsch.* **35a**, 350.
 Heyland, G. R., Charlton, M., Griffith, T. C., and Wright, G. L. (1982). *Can. J. Phys.* **60**, 503.
 Huxley, L. G. H., and Crompton, R. W. (1974). 'The Diffusion and Drift of Electrons in Gases' (Wiley: New York).

- Lee, G. F., and Jones, J. (1974). *Can. J. Phys.* **52**, 17.
- Lee, G. F., Orth, P. H. R., and Jones, G. (1969). *Phys. Lett. A* **28**, 674.
- McEachran, R. P., Ryman, A. G., and Stauffer, A. D. (1978). *J. Phys. B* **11**, 551.
- McEachran, R. P., Ryman, A. G., and Stauffer, A. D. (1979). *J. Phys. B* **12**, 1031.
- McEachran, R. P., and Stauffer, A. D. (1977). *J. Phys. B* **10**, 663.
- McEachran, R. P., Stauffer, A. D., and Campbell, L. E. M. (1980). *J. Phys. B* **13**, 1281.
- Orth, P. H. R., and Jones, G. (1969). *Phys. Rev.* **183**, 7.
- Schrader, D. M., and Svetic, R. E. (1982). *Can. J. Phys.* **60**, 157.
- Sinha, K. V., and Grover, P. S. (1985). *Ind. J. Pure Appl. Phys.* **23**, 493.

Manuscript received 11 December 1985, accepted 24 March 1986

