



Analyzing of Transport Phenomena using Transport Equation

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ABSTRACT

The numerical solution of the transport equation was utilized to study the transport phenomena. The currents and transport coefficients such as, the diffusivity, the electrical conductivity, the thermal conductivity and Wiedemann-Franz Law in addition of investigating the Einstein relation which calculated from the equations (23-25) and (27-37) respectively at 300°K for values $E/N=(0.5,1,2,3,4,5)\times 10^{-16}$ V.cm² and $(1,2,4,6,8,10)\times 10^{-18}$ V.cm² for nitrogen and argon gases respectively. The results reveals to the agreement with the publisher lectures.

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1. Introduction

The analysis of transport phenomena within system that used density and temperature gradients by using the Boltzmann transport equation is a powerful tool. The transport equation was applied to analyze of the diffusion coefficient, relationship between them, and the general currents within a system.

2. Transport Equation Derivation

Assume the system contains in each place a local rang, which is the thermal velocities taken by an equilibrium equation distribution function, where the temperature is depended and varies from place to place at the system with non-uniform particle density and temperature, nevertheless, a non-equilibrium distribution function determines the probability of a particle within the system. The transport equation enables application of properties of equilibrium system to study the non-equilibrium system.

Assume the medium contains the randomly moving particles with a temperature gradient with the x-axis at an angle θ at instant the particle collides with the medium, after the collision the thermal velocity v of the particle will be $f_o(x, T(x))$ at the collision point as shown in Figure [1,2,3].

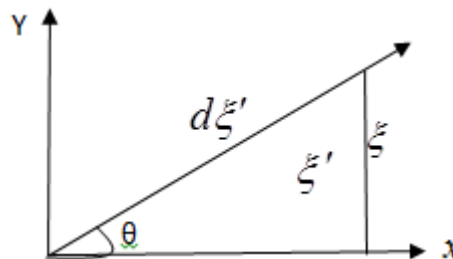


Figure 1. Moving of particle within a medium in a ξ direction.

The projection of ξ on the axis is:

$$\Delta x = \Delta \xi \cos(\theta) \quad (1)$$

the particle probability dp , that collides with the medium is proportional to $d\xi$, n_s and σ_s :

$$dp = -pd\xi \sum n_s \sigma_s \quad (2)$$

Where

$$\sum n_s \sigma_s = \frac{1}{\lambda} \quad (3)$$

Substitute equation (3) into (2) yields:

$$dp = -\frac{pd\xi}{\lambda} \quad (4)$$

where $d\xi$ refer the distance element which is the particle travelled through the medium, n_s refers to the density of scattering centers, σ_s refers the scattering cross section, the sum over S account for all different types centers and λ refers the mean free path.

The last collision of the particle before reaching cross section plane at ξ was along $d\xi'$ at position $\xi'(\xi > \xi')$, therefore, probability according to the above equations is:

$$\frac{P(\xi')d\xi'}{\lambda} = \frac{\exp(\xi' - \xi)d\xi'}{\lambda} \quad (5)$$

since

$$\frac{\int_{-\infty}^{\xi} (\xi' - \xi) \cdot P(\xi') d(\xi')}{\lambda} = \lambda$$

this mean, λ , is the probable distance which the particle travelers through the medium.

At adding the local velocity distribution at all $d\xi$ along the line up to ξ would be obtain the particle velocity distribution ν , at the cross section plane ξ , wherefore each distribution is multiplied by the probability that the particle comes from that distance, equation(5) gives:

$$F(\xi, \nu) = \frac{\int_{-\infty}^{\xi} f_o(\xi', \nu) P(\xi') d\xi'}{\lambda} \quad (6)$$

where $\nu = |\mathbf{V}|$ and $f_o(\xi', \nu)$ were the local equilibrium distribution at ξ' . It will be use the first terms of Taylor series, when the equilibrium distribution does not change along the mean free bath λ which is:

$$f_o(\xi', \nu) = f_o(\xi, \nu) + \frac{\partial f_o}{\partial \xi} (\xi' - \xi) + \frac{\partial f_o}{\partial \nu} [\nu(\xi') - \nu(\xi)] \quad (7)$$

The acting of force on the particle caused the change in velocity, such as the electric field or gravitation field for a change particle considers the force acts in x-axis, hence the velocity change gives:

$$\begin{aligned} \nu(\xi')^2 - \nu(\xi)^2 &\approx 2\nu(\nu' - \nu) \\ &= 2a(\xi' - \xi)\cos(\theta) \end{aligned} \quad (8)$$

$$a = \frac{eE}{m}$$

where m refers to the particle acceleration, E is the electric field. Substituting equation (8) and equation (7) into equation (6), integrating over ξ' , and finally substituting χ and θ for ξ according to equation (1) yields:

$$f(x, \nu, \theta) = f(x, \nu) - \lambda \cos(\theta) \left\{ \frac{\partial f_o}{\partial x} + \left(\frac{a}{\nu} \right) \frac{\partial f_o}{\partial \nu} \right\} \quad (9)$$

equation (9) is the non-equilibrium distribution and called the linear Boltzmann transport equation in a somewhat non-traditional form. The distribution $f_o(x, \nu)$ is the local equilibrium distribution which is given by Maxwell-Boltzmann or Fermi-Dirac distribution. The external forces and medium properties enter through the acceleration a and mean free path λ respectively. The general form of equation (9) is :

$$\frac{\partial f}{\partial t} + \nu \Delta_{\chi} f + a \nabla_{\nu} f = \frac{(f_o - f)}{\tau} \quad (10)$$

which is including a constant relaxation time τ .

where

$$\tau = \frac{\lambda}{\nu} \quad (11)$$

3. Particles Currents

The particle moves through the medium will cross a plane section at χ during Δt with a velocity \underline{v} if its distance from the plane is less than $|\underline{v}| \cos(\theta) \Delta t$ [2,3,4]. Hence the current of the particle is obtained by summing all the velocity of all directions is space according to the distribution probability for each velocity which is:

$$J_n = 2\pi \int \int f(x, v, \theta) |\underline{v}| v^2 \cos(\theta) \sin(\theta) d\theta dv \quad (12)$$

substitute the equation (9) into Equation(12) gives :

$$J_n = \int \int f_o(x, v) |\underline{v}| \cos(2\pi v^2) dv \sin(\theta) d\theta - \int \lambda \frac{\partial f_o}{\partial \chi} |\underline{v}| 2\pi v^2 \cos^2(\theta) \sin(\theta) d\theta - \int \int \lambda \frac{a}{v} \frac{\partial f_o}{\partial v} |\underline{v}| 2\pi v^2 dv \cos^2(\theta) \sin(\theta) d\theta \quad (13)$$

where $f_o(x, v) = 0$ as indicator in equation(9), and $\int \cos^2 \theta \sin \theta d\theta = \frac{2}{3}$, hence equation(13) gives:

$$\begin{aligned} J_n &= 0 - \frac{4\pi\lambda}{3} \int \frac{\partial f_o}{\partial x} |\underline{v}| v^2 dv - \frac{4\pi\lambda}{3} \int \frac{a}{v} \frac{\partial f_o}{\partial v} |\underline{v}| v^2 dv \\ &= 0 - \frac{4\pi\lambda}{3} \left[\int \frac{\partial f_o}{\partial x} |\underline{v}| v^2 dv + \int \frac{a}{v} \frac{\partial f_o}{\partial v} |\underline{v}| v^2 dv \right] \\ &= -\frac{4\pi\lambda}{3} \left[\int \frac{\partial f_o}{\partial x} v^3 dv + \frac{eE}{m} \int \frac{\partial f_o}{\partial v} v^2 dv \right] \end{aligned} \quad (14)$$

where J_n is called the particle current .

From the above with each particle there is energy associated with it, u which is :

$$U = \frac{1}{2} m v^2$$

since the energy current J_u and according to the probability of the distribution becomes:

$$J_u = m\pi \int \int f(x, v, \theta) |\underline{v}|^3 v^2 dv \cos(\theta) \sin(\theta) d\theta \quad (15)$$

substitution of the distribution function equation(9) into equation(15) gives :

$$\begin{aligned} u &= m\pi \int \left[f_o(x, v) - \lambda \cos(\theta) \left(\frac{\partial f_o}{\partial x} + \frac{a}{v} \frac{\partial f_o}{\partial v} \right) |\underline{v}|^3 v^2 dv \cos(\theta) \sin(\theta) d\theta \right] \\ &= m\pi \int f_o(x, v) |\underline{v}|^3 v^2 dv \cos(\theta) \sin(\theta) - m\pi \int \lambda \frac{\partial f_o}{\partial x} |\underline{v}|^3 v^2 dv \cos^2 \theta \sin(\theta) d\theta \\ &= m\pi \int \lambda \frac{a}{v} \frac{\partial f_o}{\partial x} |\underline{v}|^3 v^2 dv \cos^2(\theta) \sin(\theta) d\theta \end{aligned} \quad (16)$$

from equation(9), $f_o(x, v) = 0$ and the trigonometric integral is:

$$\int \cos^2 \theta \sin \theta d\theta = \frac{2}{3}, \text{ wherefore, equation(16) gives:}$$

$$J_u = \frac{4\pi\lambda}{3} \left[\int \frac{\partial f_o}{\partial x} v dv + \frac{eE}{m} \int \frac{\partial f_o}{\partial v} v^4 dv \right] \quad (17)$$

$$a = \frac{eE}{m}$$

where m and J_u is called the energy current .

when applied the Maxwell-Boltzmann distribution you can calculate the currents as follow :

$$f_o(x, u) = n(x) \left(\frac{m}{2\pi kT} \right)^{\frac{3}{2}} \exp \left(-\frac{mv^2}{2kT} \right) \quad (18)$$

where $n(x)$ refers to the particle density. Using the normalization condition to

$n(x)$ refers to the particle density. Using the normalization condition to calculate the pre-exponential factor indicators in equation(18), which is :

$$\int_0^{\infty} 4\pi v^2 f_o dv = n$$

from equation (18) gives :

$$\frac{\partial f_o}{\partial v} = n(x) \left(\frac{m}{2\pi kT} \right)^{\frac{3}{2}} \exp\left(-\frac{mv^2}{2kT}\right) \left(-\frac{mv}{kT}\right)$$

(19)

(20)

$$\frac{\partial f_o}{\partial x} = \left(\frac{m}{2\pi kT} \right)^{\frac{3}{2}} \exp\left(-\frac{mv^2}{2kT}\right) n(x)$$

equations (14,18,19 and 20) were obtained:

$$\begin{aligned} J_n &= -\frac{4\pi\lambda}{3} \left[\int \frac{\partial f_o}{\partial x} v^3 dv + \frac{eE}{m} \int n(x) \left(\frac{m}{2\pi kT} \right)^{\frac{3}{2}} (-) \exp\left(-\frac{mv^2}{2kT}\right) \frac{2mv}{2kT} v^2 dv \right] \\ &= -\frac{4\pi\lambda}{3} \left[\int \frac{\partial f_o}{\partial x} v^3 dv - \frac{eE}{m} \int n(x) \left(\frac{m}{2\pi kT} \right)^{\frac{3}{2}} \frac{m}{kT} \exp\left(-\frac{mv^2}{2kT}\right) v^3 dv \right] \\ &= -\frac{4\pi\lambda}{3} \left[\int \frac{\partial f_o}{\partial x} v^3 dv - \frac{eE}{m} \int n(x) \left(\frac{m}{2\pi kT} \right)^{\frac{3}{2}} \exp\left(-\frac{mv^2}{2kT}\right) v^3 dv \right] \\ &= \frac{4\pi\lambda}{3} \left[-\int \frac{\partial f_o}{\partial x} v^3 dv + \frac{eE}{m} \int n(x) \left(\frac{m}{2\pi kT} \right)^{\frac{3}{2}} \exp\left(-\frac{mv^2}{2kT}\right) v^3 dv \right] \\ &= \frac{4\pi\lambda}{3} \left[-\int \frac{\partial f_o}{\partial x} v^3 dv + \frac{eE}{m} \int f_o v^3 dv \right] \\ &= \frac{4\pi\lambda}{3} \left[\frac{eE}{kT} \int f_o v^3 dv - \int \frac{\partial f_o}{\partial x} v^3 dv \right] \end{aligned}$$

(21)

from equation(21) obtained the integral:

$$\begin{aligned} \int f_o v^3 dv &= \int n(x) \left(\frac{m}{2\pi kT} \right)^{\frac{3}{2}} \exp\left(-\frac{mv^2}{2kT}\right) v^3 dv \\ &= \frac{n}{\pi} \left(\frac{kT}{2\pi m} \right)^{\frac{1}{2}} \end{aligned}$$

(22)

substitute the equation (22) into equation (21) gives:

$$\begin{aligned} J_n &= \frac{4\pi\lambda}{3} \left(\frac{eE}{kT} - \frac{d}{dx} \right) \frac{n}{\pi} \left(\frac{kT}{2\pi m} \right)^{\frac{1}{2}} \\ &= \frac{4\lambda}{3(2\pi m)^{\frac{1}{2}}} \left[\frac{eEn}{(kT)^{\frac{1}{2}}} - \frac{d}{dx} \left(n(kT)^{\frac{1}{2}} \right) \right] \end{aligned}$$

(23)

by mathematical simplify according to the above gives :

$$J_u = \frac{8\lambda}{3(2\pi m)^{\frac{1}{2}}} \left[(kT)^{\frac{1}{2}} eE - \frac{d}{dx} \left\{ n(kT)^{\frac{3}{2}} \right\} \right]$$

(24)

the relation between equation(23) and equation(24) gives:

$$J_u = 2k \left\{ TJ_n - \frac{4\lambda}{3} \left(\frac{kT}{2\pi m} \right)^{\frac{1}{2}} n \frac{dT}{dx} \right\}$$

this equation is proportional to the temperature gradient and independent of the particle current; The energy current J_u is a sum of convection term and the heat conduction term .

The charge density does not depend on the temperature in case of the electrical conductors but not in semiconductors, wherefore the electrical current J_q from equation (23) becomes:

$$J_q = eJ_n = \frac{4\lambda e^2 n}{3(2\pi m T)^{\frac{1}{2}}} \left(E - \frac{k}{2e} \frac{dT}{dx} \right) \quad (26)$$

Transport Parameters:

A – The diffusivity D [5, 6, and 7], from equation (23) yields:

$$J_n = \frac{4\lambda(kT)^{\frac{1}{2}}}{3(2\pi m)^{\frac{1}{2}}} \left[\frac{eEm(kT)^{\frac{1}{2}}}{(kT)^{\frac{3}{2}}} - \frac{dn}{dx} \right] \quad (27)$$

at, $\frac{dT}{dx} = 0$, $E=0$, yields:

$$J_n = - \frac{4\lambda(kT)^{\frac{1}{2}}}{3(2\pi m)^{\frac{1}{2}}} \frac{dn}{dx} \quad (28)$$

where,

$$D = \frac{4\lambda}{3} \left(\frac{kT}{2\pi m} \right)^{\frac{1}{2}} \quad (29)$$

substitution equation (29) into equation(28) gives:

$$J_n = -D \frac{dn}{dx}$$

Equation (29) is called the diffusivity D. The electrical conductivity was obtained from equation (26) and equation (27) give:

$$J_q = eJ_n, \text{ at } \frac{dT}{dx} = 0, \text{ and } \frac{dn}{dx} = 0,$$

$$J_q = \frac{4\lambda e^2 n E}{3(2\pi m T)^{\frac{1}{2}}} \quad (30)$$

$$J_q = \sigma E \quad (31)$$

where

$$\sigma = \frac{4\lambda e^2 n}{3(mkT)^{\frac{1}{2}}} \quad (32)$$

$$\lambda = \frac{\bar{v}}{2.39 \times 10^{-9} n K_1} \quad (33)$$

$$K_1 = \frac{e D}{kT \mu} \quad (34)$$

$$\bar{v} = \left(\frac{8kT}{\pi m} \right)^{\frac{1}{2}} \quad (35)$$

hence σ was called the electrical conductivity.

From the equation (25), at $J_n=0$ gives:

$$J_u = -\frac{8\lambda}{3} \left(\frac{kT}{2\pi m} \right)^{\frac{1}{2}} nk \frac{dT}{dx}$$

$$J_u = -k \frac{dT}{dx}$$

where

$$K = \frac{8\lambda}{3} \left(\frac{kT}{2\pi m} \right)^{\frac{1}{2}} nk \quad (36)$$

where K is called the thermal conductivity .By comparing these coefficient yields:

$$\frac{K}{\sigma} = 2kT \left(\frac{k}{e} \right)^2 \quad (37)$$

where $\frac{K}{\sigma}$ is called the wiedemann-Franz law,

and another formula is :

$$\frac{D}{\mu} = \frac{D}{\left(\frac{\sigma}{ne} \right)} \quad (38)$$

this equation is called Einstein relation.

5 - Calculations of E, D/ μ ,L

For the electron distribution function $f(v,r,t)$, considering elastic collision only. From a two term expansion of Boltzmann's equation in an expansion of f using spherical harmonics about the direction f_1 in velocity space. The truncated expansion:

$$f(v,r,t) = f_o(v,r,t) + \frac{V}{v} \cdot f_1(v,r,t) \quad (39)$$

according to the equation (1), the Boltzmann equation take the form [8, 9,and 10]:

$$\left(\frac{\partial f_o}{\partial t} \right) + \frac{1}{3} v \nabla \cdot f_1 + \left(\frac{e}{3m v^2} \right) \left(\frac{\partial}{\partial v} \right) (v^2 E \cdot f_1) = \left(\frac{1}{2v^2} \right) \left(\frac{\partial}{\partial v} \right) \quad (40)$$

$$\left[v^2 \delta v(v,r) \cdot \left\{ \left(\frac{kT_g}{m} \right) \left(\frac{\partial f_o}{\partial t} \right) + v f_o \right\} \right] + S_{o,e}(f_o)$$

$$\frac{\partial f_1}{\partial t} + v \nabla f_o + \frac{eE}{m} \frac{\partial f_o}{\partial v} + \frac{e}{m} (B \times f_1) = -v(v,r) f_1 - S_{1,e}(f_1) \quad (41)$$

where v refers to the electron velocity , ∇ , refers to the operator e refers to the electronic charge (negative number), m is the electron mass, M is the ion or neutral particle mass, E is the applied electric field, k is the Boltzmann's constant, T_g is the gas temperature, B is the magnetic field, δ is equal to $2m/M$, $v(v,r)$ is the collisions frequency for momentum transfer between electron and heavy particles $s_{o,e}$ refers to the zeroth -order electron-electron collision term and $s_{1,e}$ refers to the first-order electron-electron collision term.

The solution of the Boltzmann transport equation was yield the transport coefficients such as, the electric field E , and the ratio of the diffusion coefficient to the mobility D/μ . From equations (33) and (34) were utilized to get the mean free path λ .

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6. Conclusion

- A-** The general currents in a medium with particle were calculated by using the numerically solution of the Boltzmann transport equation.
- B-** The calculation of the transport coefficient such as, electric thermal conductivity and diffusivity were verified the wiedemann-Fraz and Einstein law.
- C-** Boltzmann transport equation expresses the non-equilibrium distribution in terms of local equilibrium distribution, which is the transport equation enables application of properties of equilibrium systems.
- D-** The equation can describe macroscopic phenomena, such as the electrical conductivity, Hall effect and diffusion process.
- E-** The equation has properly generalized, for other systems such as, electron transport, photon transport in super fluids and radiative transport in planetary.
- F-** The equation still has much use and applicability.

7. Results and Discussion

From the currents in the equation (23-25) are calculation directly, the transport coefficients and currents at 300 k°.

Figure (2) was showing the increasing of the diffusivity with mean free path i.e., the mean free path between the collisions is large.

Figure (3) appears the electrical current was increase with mean free path but decreased with the mean free path as showing in figure(4).

Figure (5) was showing the electrical current decreased with electrical field, but it was increasing with electrical field in form ramp as showing in figure (6).

Figure(7) was offer the increasing of the electrical current with the electrical conductivity, otherwise decrease with electrical conductivity as seen in figure(8).

Figure(9) and(10) were brought out that the electrical conductivity and the thermal conductivity are increasing with mean free path respectively.

Figure(11) and (12) were referred that diffusivity to the mobility were constant with increasing of the diffusivity and electrical conductivity respectively. These figures were implemented the Wiedmann-Franz law, which is:

$$\frac{K}{\sigma} = 2kT \left(\frac{K}{e} \right)^2$$

and Einstein relation which is:

$$\frac{D}{\mu} = \frac{Dne}{\sigma} = \frac{kT}{e}$$

by comparing these coefficients which are diffusivity, electrical conductivity and thermal conductivity.

Figure (13) was seen that the Townsend's energy factor was increased with the diffusivity to the mobility ratio.

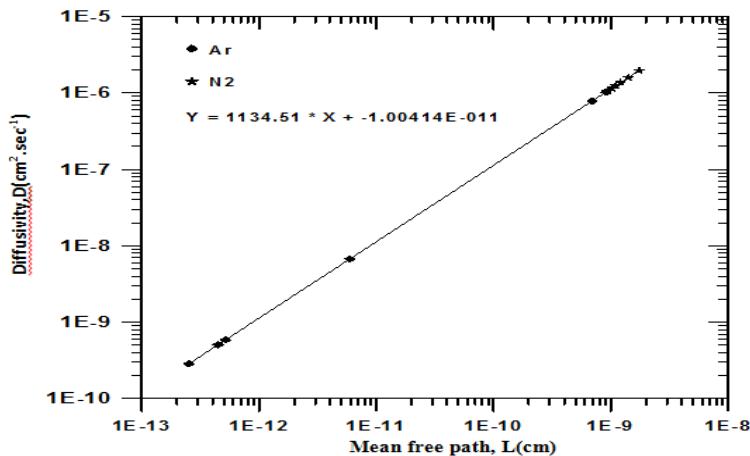


Fig 2 . The diffusivity,D, versus the mean free path, L, for the gases N₂ and Ar.

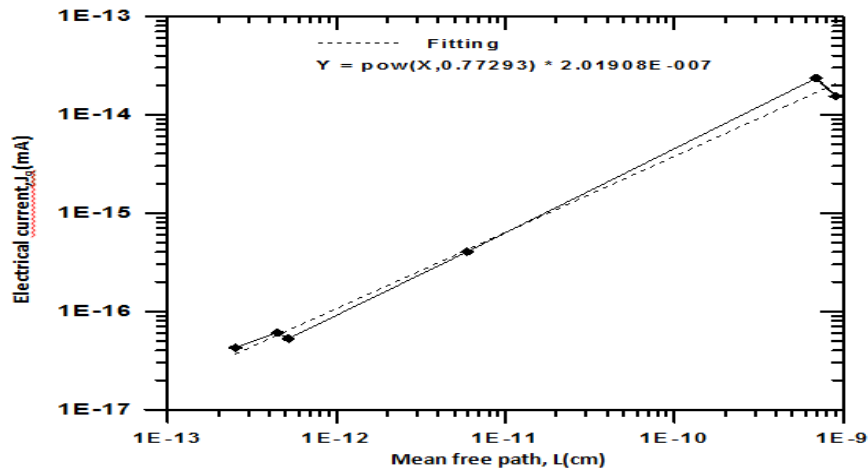


Fig 3. The electrical current, J_q , as a function of the mean free path, L , for the gas Ar.

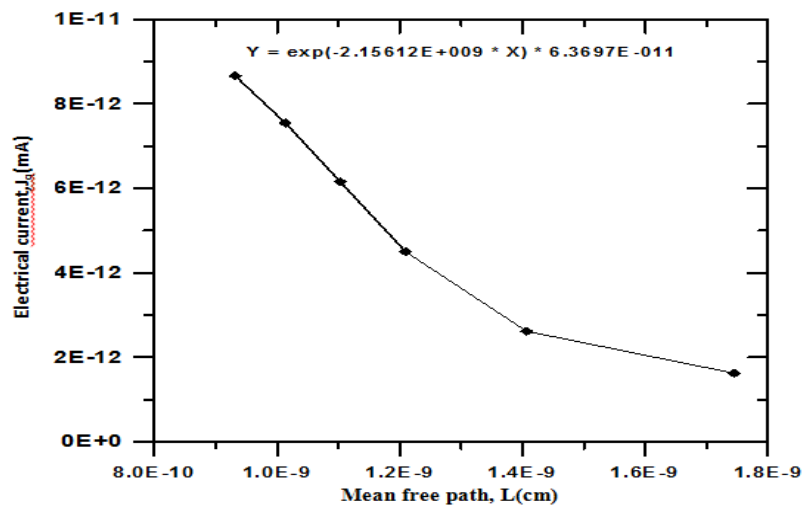


Fig 4. The electrical current, J_q , as a function of the mean free path, L , for the Nitrogen gas, N_2 .

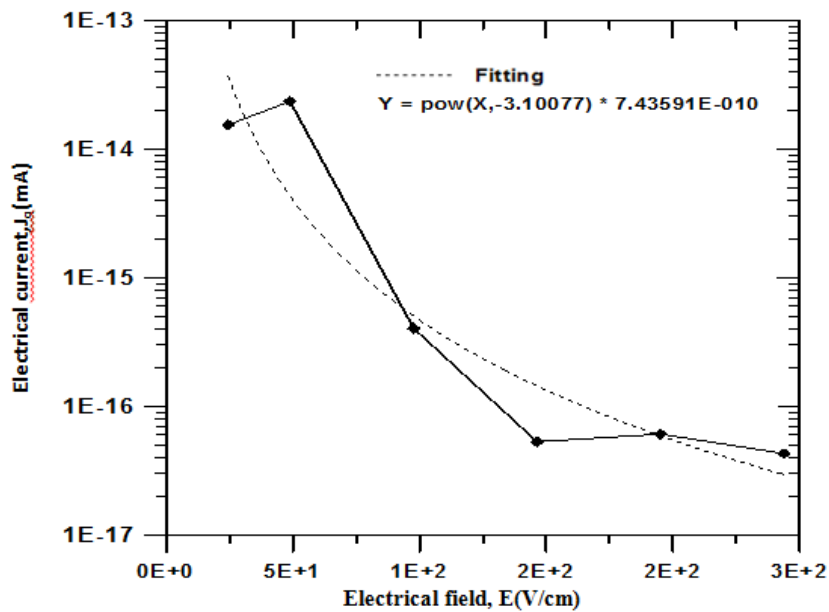


Fig 5 . The electrical current, J_q , as a function of the electrical field, E , for the Argon gas, Ar.

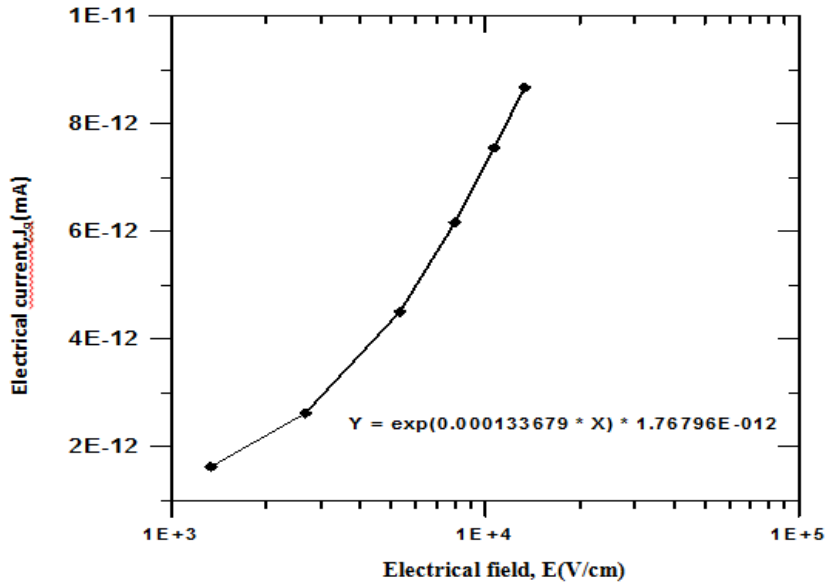


Fig 6 . The electrical current, J_q , as a function of the electrical field, E , for the Nitrogen gas, N_2 .

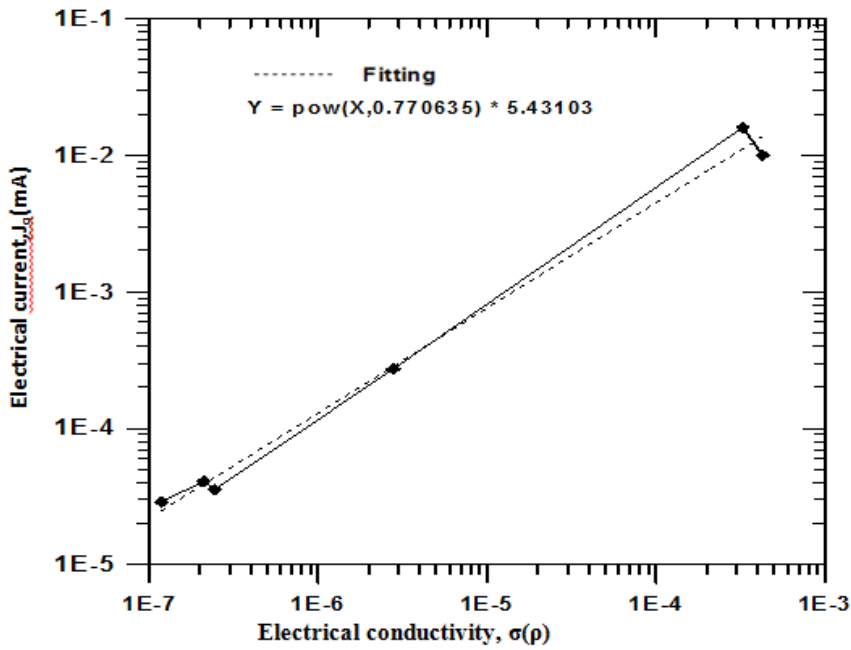


Fig 7. The electrical current, J_q , as a function of the electrical conductivity, $\sigma(\rho)$, for the Argon gas, Ar.

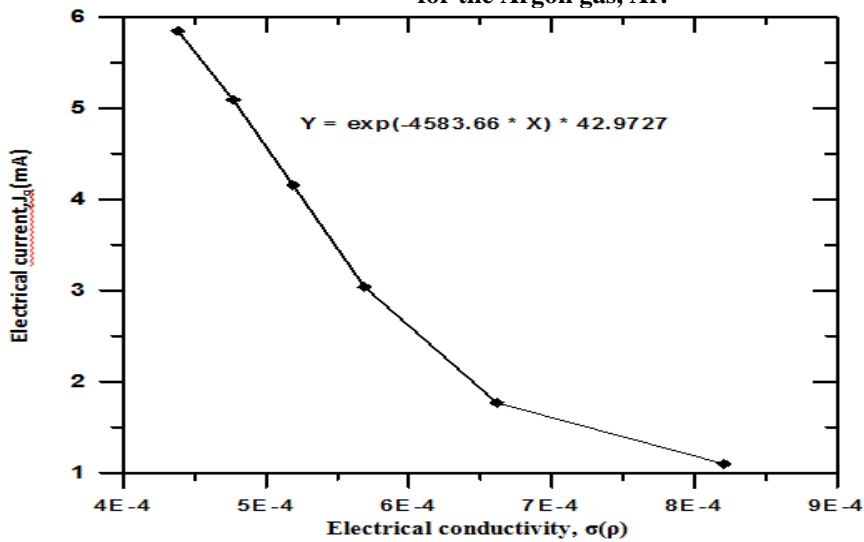


Fig 8. The electrical current, J_q , as a function of the electrical conductivity, $\sigma(\rho)$, for the Nitrogen gas, N_2 .

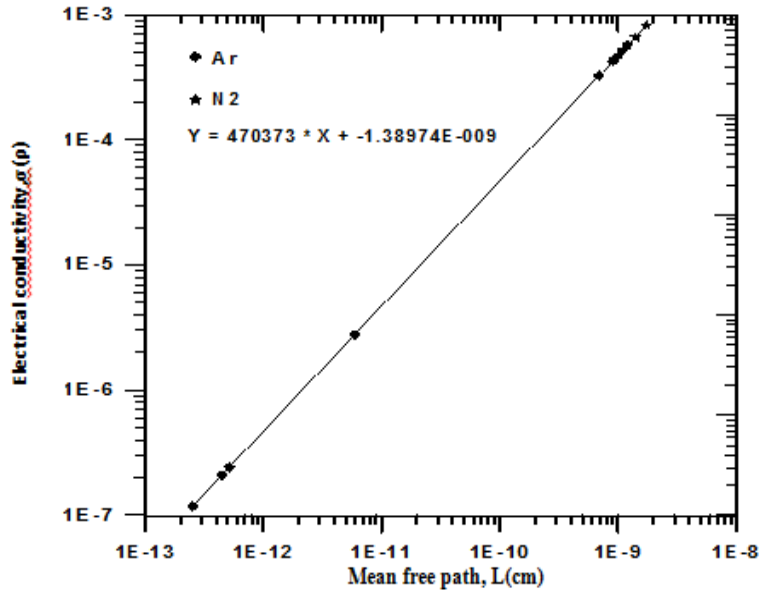


Fig 9. The electrical conductivity, σ as a function the mean free path, L for the Argon and Nitrogen gases.

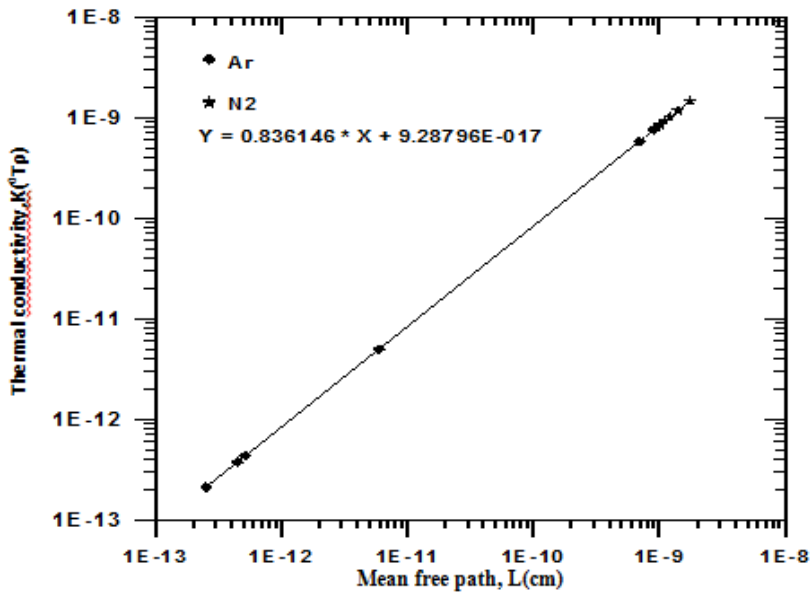


Fig 10. The thermal conductivity, K as a function the mean free path, L for the Argon and Nitrogen gases.

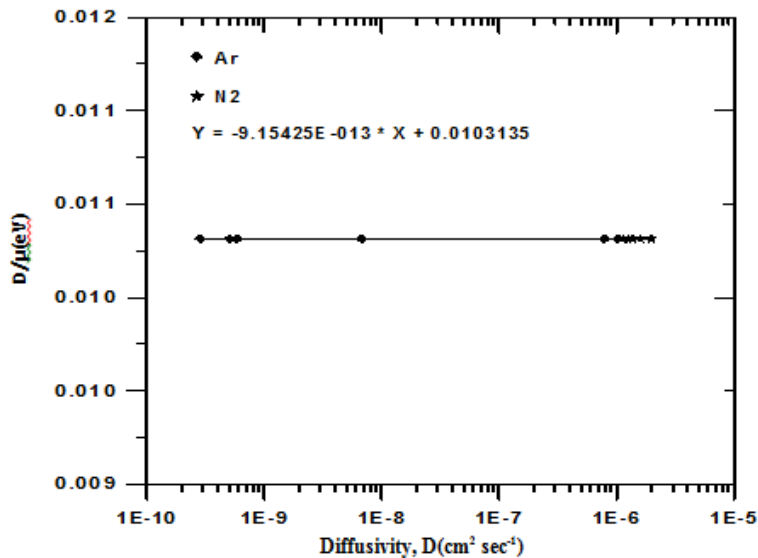


Fig 11. The diffusivity to the mobility, D/ μ , ratio as a function of the diffusivity for the Argon and Nitrogen gases.

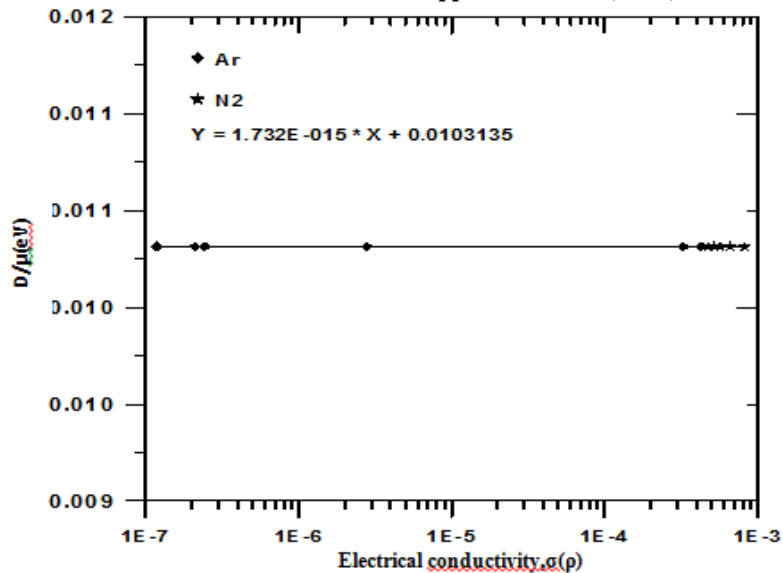


Fig 12 . The diffusivity to the mobility, D/μ , ratio as a function of the electrical conductivity, σ for the Argon and Nitrogen gases.

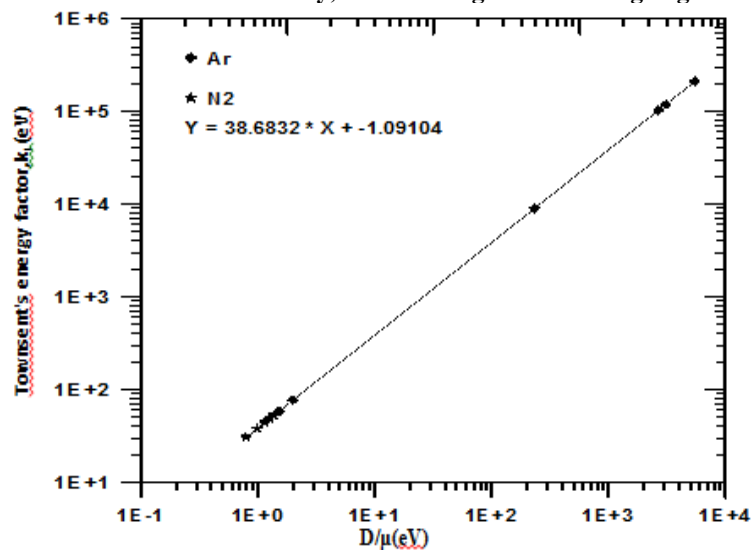


Fig 13. The Townsend's energy factor, k , as a function of the diffusivity to the mobility, D/μ ratio for the Argon and Nitrogen gases.

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