Determination of Maxwell-Boltzmann Distribution Probability for (^{40}Ar, ^{4}He and N_2) in Gases

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Abstract

In this work we have constructed a theoretical model to calculate the Maxwell-Boltzmann distribution for gases and typical speeds of electrons which are: the most probable speed υ_p, the mean speed $<\upsilon>$, and the root-mean-square speed υ_{rms}, had been carried out .Further more satisfies the condition of speed for Nitrogen , Argon , and Helium gases at 300°K for ranges [E/N=(0.5,1,2,3,4,5)×10^{-16} ; (1,2,4,6,8,10) ×10^{-18}; (0.1214, 0.182, 0.455, 1.214, 1.82, 4.55, 12.14, 18.2, 24.3, 30.3) ×10^{-18}] (V cm^2) respectively.

we get a good agreement between the results which obtained by our theoretical model and the experimental results for different researchers . These results had been plotted as functions with their variables.

Keyword: Boltzmann equation, Collision cross-section, Charged particle transport, Swarm parameters.

Introduction

The Maxwell-Boltzmann distribution explains the probability of a particles speed being near a given value as a function of the temperature of the system , the mass of the particle and that speed value. This probability distribution is named after James Clerk Maxwell and Ludwing Boltzmann. The statistical behavior of many particle systems is described by the product of the density of states and the distribution function for these states. One of the simplest cases is that for radioactive decay since you are dealing with pure probability. The density of states can just be taken as a constant since there is no preference for one decay time over another, and the distribution function is simply

$N=N_o e^{-t/\tau}$

where τ refers to the average lifetime.

There are many physicals applications of the distribution functions ,such as, tell us that the probability that any one molecule is highly unlikely to grab much more than it average share of the total energy available to all the molecules, applies to ideal gases close to thermodynamic equilibrium[1-4] .

Theory detection

The Maxwell-Boltzmann distribution can be derived from the Boltzmann distribution for energies using kinetic theory , but the derivation at the beginning by Maxwell, supposed all three directions in the same fashion [1].

$$\frac{N_i}{N} = \frac{g_i \exp(-E/KT)}{\sum_j g_j \exp(-E_j/KT)} \tag{1}$$

$$\frac{N_i}{N} = \frac{1}{Z}\exp\left[\frac{P_x^2 + P_y^2 + P_z^2}{2mKT}\right] \tag{2}$$

where

$$E = P^2/2m \tag{3}$$

$p_x, p_y, p_z]$ (4)

and

$$\frac{N_i}{N} \alpha f_p \tag{5}$$

Therefore where

$$f_p(p_x, p_y, p_z) = \frac{c}{Z}\exp\left[\frac{-p_x^2 + p_y^2 + p_z^2}{2mKT}\right] \tag{6}$$

$$c = Z\frac{2}{(\pi m K T)^{3/2}} \tag{7}$$

hence

$$f_p(p_x, p_y, p_z) = \left(\frac{1}{2\pi m K T}\right)^{3/2} \exp\left[\frac{-p_x^2 + p_y^2 + p_z^2}{mKT}\right] \tag{8}$$

whereas N_i refers to the number of molecules at equilibrium temperature T, in state i which has energy E_i and degeneracy g_i , N is the total number of molecules in the system and k is the Boltzmann constant .The denominator in this equation is known as the canonical partition function, p refers to the momentum vector, Z refers to the partition function, m refers to the electron mass,

Distribution for the speed

The Maxwell-Boltzmann distribution are more interested in the speeds of molecules rather than their component velocities which take the form:

$$f(v) = 4\pi\left(\frac{m}{2\pi KT}\right)^{3/2} v^2 \exp\left[\frac{-m(v_x^2 + v_y^2 + v_z^2)}{2KT}\right] \tag{9}$$

Since speed V, is :

$$V = (v_x^2 + v_y^2 + v_z^2)^{1/2} \tag{10}$$

Substitute Eq.(10) into Eq.(9) gives :

$$f(v) = 4\pi\left(\frac{m}{2\pi KT}\right)^{3/2} v^2 \exp\left[\frac{-mv^2}{2KT}\right] \tag{11}$$

the unit of f(v) is sec/cm (reciprocal speed) (1/speed).

This distribution is a Maxwell-Boltzmann distribution with a = mKT

Distribution for relative speed

The relative speed is defined as :

$$u = \frac{v}{v_p} \qquad (12)$$

Since

$$v_p = \left(\frac{2KT}{m}\right)^{1/2} = \left(\frac{2RT}{m}\right)^{1/2} \qquad (13)$$

Eq.(13) is called the most probable speed , v_p .

Typical speeds

A- The most probable speed v_p , is the speed most likely by any molecule (of the same mass m) in the system and corresponds to the maximum value or mode of f(v) . To find it : we calculate df/dv , set it to zero and solve for v , from Eq.(11) and Eqs.(12-13)

$$\frac{df\ (v)}{dv} = 0$$

Which gives:

$$v_P = \left(\frac{2KT}{m}\right)^{1/2} \qquad (14)$$

B. the mean speed $<v>$ is the mathematical average of the speed distribution , which is :

$$< v >= \int_0^\infty v f(v) dv = \left(\frac{8KT}{\pi m}\right)^{1/2} \qquad (15)$$

C- The root mean square speed, v_{rms} is the square root of the average squared speed:

$$v_{rms} = \left(\int_0^\infty v^2 f(v) dv\right)^{1/2} = \left(\frac{3KT}{m}\right)^{1/2} \qquad (16)$$

the typical speeds are related as follows:

$$v_p \langle < v > \langle v_{rms} \qquad (17)$$

Computational Procedures:

Firstly: Solution of the transport equation

We suppose the electron swarm in an applied uniform electric field E, the steady – state f^o distribution written as [5-6]:

$$\frac{1}{2v^2}\frac{\partial}{\partial v}\left\{Gv_m v^3\left[f^o+\left\{\frac{KT_g}{m}+\frac{2}{3G}\left(\frac{eE}{mv_m}\right)^2\right\}\frac{1}{v}\frac{\partial f^o}{\partial v}\right]\right\}+\frac{1}{3}\frac{\partial}{\partial z}\left[\frac{eE}{mv_m}v\frac{\partial f^o}{\partial v}+\frac{1}{v^2}\frac{\partial}{\partial v}\left(\frac{eE}{mv_m}v^3 f^o\right)\right]$$
$$+\frac{v^2}{3v_m}\nabla_r^2 f^o=0 \qquad (18)$$

since field E along the negative Z-axis direction , v is the electron velocity . G is the energy loss factor, ν_m is the momentum transfer collision frequency k is the Boltzmann factor, T_g is the gas temperature which is 300K, e is the coloumbic charge. This represents integro differential equation solved numerically using the finite difference method with energy interval 0.01eV .

Secondly : Calculations of <u> ,D/μ, ν_m , and V_d parameters

The classical theory of transport processes is based on the Boltzmann transport equation . The equation can be derived simply by defining distribution function. From this equation many important results can be derived[7-8].

After solved numerically Eq.(18) had been obtained the parameters namely , electron average energy, <u> , the ratio of the diffusion coefficient to the electron mobility**,** D/μ, the momentum transfer collision frequency, ν_m , and drift velocity V_d, [9-10].These parameters could be fed to the following calculations:

From the definition of the momentum , p , for three components , P_x , P_y and P_z namely :

$$P^2=P_x^2+P_y^2+P_z^2 \qquad (19)$$
$$P=mv \qquad (20)$$
$$P^2=m^2v^2 \qquad (21)$$

where ν_d is the particle drift velocity corresponding to the particle velocity v, from the defining of the electron average energy , <u>, which is [11-13]

$$< u >= \frac{KT}{e}$$

$$KT = e < u > \tag{22}$$

where

$$L = 7.2 \times 10^{-9} \times \frac{V_d \sqrt{K_1}}{E/P}$$

$$K_1 = \frac{e}{K\,T_g} \frac{D}{\mu}$$

where L is the mean free path at pressure unit (mm Hg), K_1 is the Townsend energy factor and E/P is the applied electric field to the gas pressure ratio in unit of (V. cm^{-1} $Torr^{-1}$).

substitute Eqs. (19-22) into Eq.(8) gives

$$f_p(P_x, P_y, P_z) = \left(\frac{1}{2\pi\, n e < u >}\right)^{\frac{3}{2}} \exp\left[\frac{-m^2\, v^2}{2\, m e < u >}\right] \tag{23}$$

Substitute Eq.(22) into Eq.(11) yields:

$$f(v) = 4\pi\left(\frac{m}{2\pi e < u >}\right)^{3/2} v^2 \exp\left[-\frac{mv^2}{2e < u >}\right] \tag{24}$$

substitute Eq.(22) into Eqs.(14-16) are give :

$$v_p = \left(\frac{2e < u >}{m}\right)^{1/2} \tag{25}$$

$$< v >= \left(\frac{8e < u >}{\pi\, m}\right)^{1/2} \tag{26}$$

$$v_{rms} = \left(\frac{3e < u >}{m}\right)^{1/2} \tag{27}$$

After calculated the Eqs.(25-27) could be satisfied the condition which is:

$$v_p \langle < v > \langle v_{rms} \tag{28}$$

substitute Eqs.(25-27) into Eq.(24) respectively gives :

$$f(v_p) = 4\pi\left(\frac{m}{2\pi e <u>}\right)^{3/2} \frac{2e<u>}{m}\exp(-1) \tag{29}$$

$$f(<v>) = 4\pi\left(\frac{m}{2\pi e <u>}\right)^{3/2} \left(\frac{8e<u>}{\pi m}\right)\exp\left(-\frac{4}{\pi}\right) \tag{30}$$

$$f(v_{rms}) = 4\pi\left(\frac{m}{2\pi e <u>}\right)^{3/2} \left(\frac{3e<u>}{m}\right)\exp\left(-\frac{3}{2}\right) \tag{31}$$

Where $f(v_p)$,$f(<v>)$and $f(v_{rms})$are the Maxwell –Boltzmann speed distribution probability in term of the most probable speed v_p,mean speed $<v>$ and root mean square speed v_{rms}.

Results & Discussion

In this work the transport equation had been solved numerically in the gases medium. The gas parameters are obtained and compared with a good fit between available experimental results [14-17] and theoretical data.

Fig.(1-3)were represent the obtained theoretical values utilization the numerical solution of the boltzmann equation[9] to calculate the parameters V_d and $<u>$ which were agreement with the experimental values for figures 4, 6, and 7, [5,15-17] for N_2, Ar, and He respectively. These parameters were fed to the equations which are indicate in the figures.

Fig.(9) represents the probability density function f_p, as the function of the functions of the electron velocity υ, in the Argon , Helium and Nitrogen gases, whose show the values of the f_p, for these gases were decreasing with values of electron velocity υ, as in the experimental results , in Fig.5, [15].

Fig.(10)shows the probability density function f_p, was exponentially decreasing with the electron average energy $<u>$, for the above gases $<u>$, which is agreement with experimental results ,Fig.8, [16].

Fig.(11) shows the speed probability density function f(v) was increasing exponentially with increasing of the electron average energy <u> for Argon gas ,but for nitrogen increasing linearity with <u>.For helium gas the function f(v) was increasing sharply between the values, $f(v)=(3.04003\times10^{-167}-4.03473\times10^{-166})(eV)^{-3/2}$ and between the values $(4.08455-1.60648)\times10^{-166}\ (eV)^{-3/2}$ the function becomes nearly stable with <u>.

Fig.(12) shows the speed probability density function was linearity increasing with the electron velocity v, for N_2, Ar and He gases except between the values of $f(v)=(1.81511-1.43718)\times10^{-167}\ (eV)^{-3/2}$ and $(4.08455-1.60648)\times10^{-166}\ (eV)^{-3/2}$ were slowly decreasing with electron velocity , for argon and helium gases respectively.

Fig.(13) shows that the most probable speed v_p. the mean speed <v>, and the root-mean-square v_{rms} proportional increase with electron average energy, <u>, according to the condition $v_p< \langle v\rangle < v_{rms}$ and satisfies, Eq.(28).

Fig.(14) had be appeared the Maxwell-Boltzmann speed distribution probability decrease then become stable with increasing of the electron average energy,<u>. Satisfying the condition $v_p << v > < v_{rms.}$

Conclusion

1. The transport equation is solved numerically in the gaseous medium after applied electric electric field, therefore the transport parameters, electron energy average<u>, the electron diffusion coefficient to the electron mobility, momentum transport collision frequency and electron drift velocity are calculate by using computer program [9].
2. The transport parameters, which mentioned above have being fed into equations (23-31) to calculate the parameters as indicate in the figures.
3. we achieved to confirm the basic condition of equation (17) by a good agreement for variables of equations (23-31).
4. The results are show a good a agreement with the experimental values.

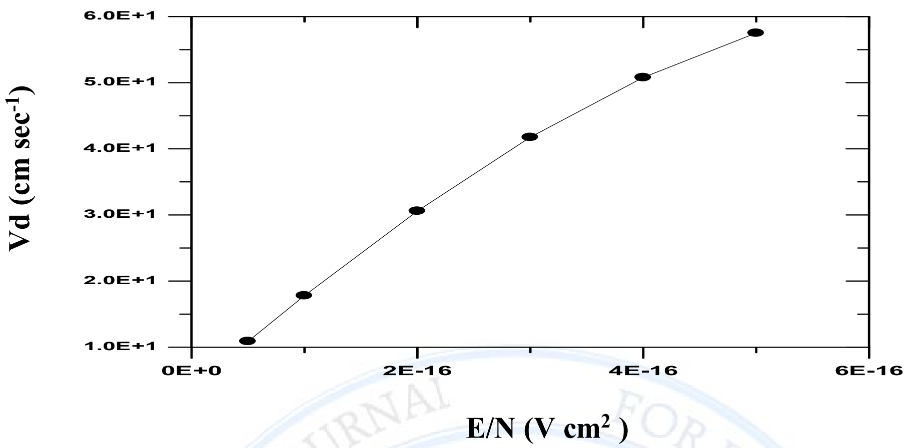


Fig. (1): The drift velocity V_d as a function of the applied electric field to the gas total number density ratio E/N for Nitrogen gas.

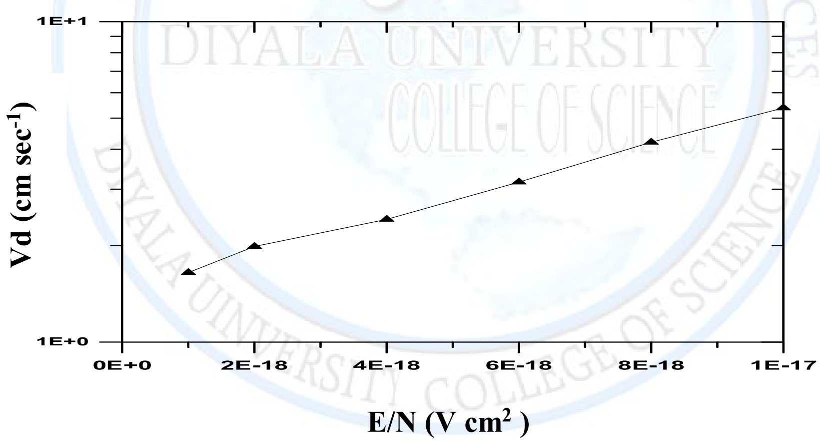


Fig. (2): The drift velocity V_d as a function of the applied electric field to the gas total number density ratio E/N for Argon gas.

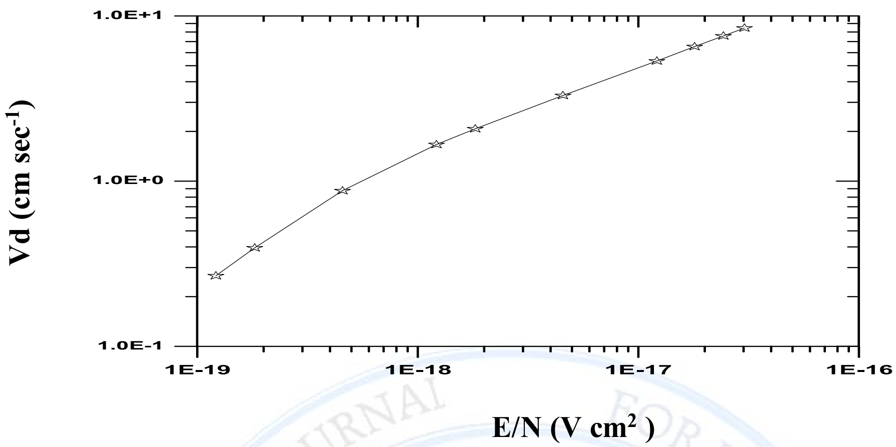


Fig. (3): The drift velocity V_d as a function of the applied electric field to the gas total number density ratio E/N for Helium gas.

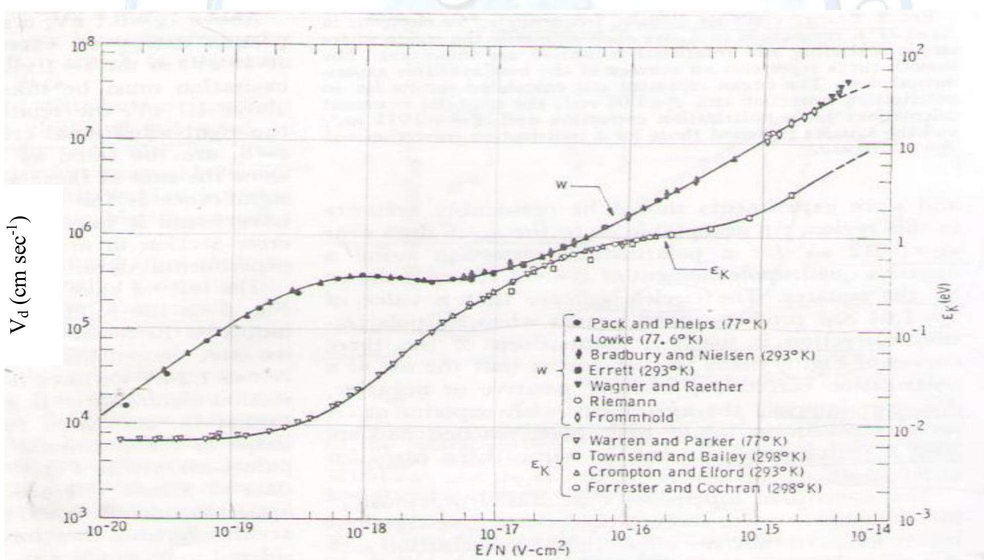


Fig. (4) : Drift velocity V_d and characteristic energy for electron in N_2 at 77^{o}K . The points represent the various experimental result and the smooth curves our computations for no polarization correction .

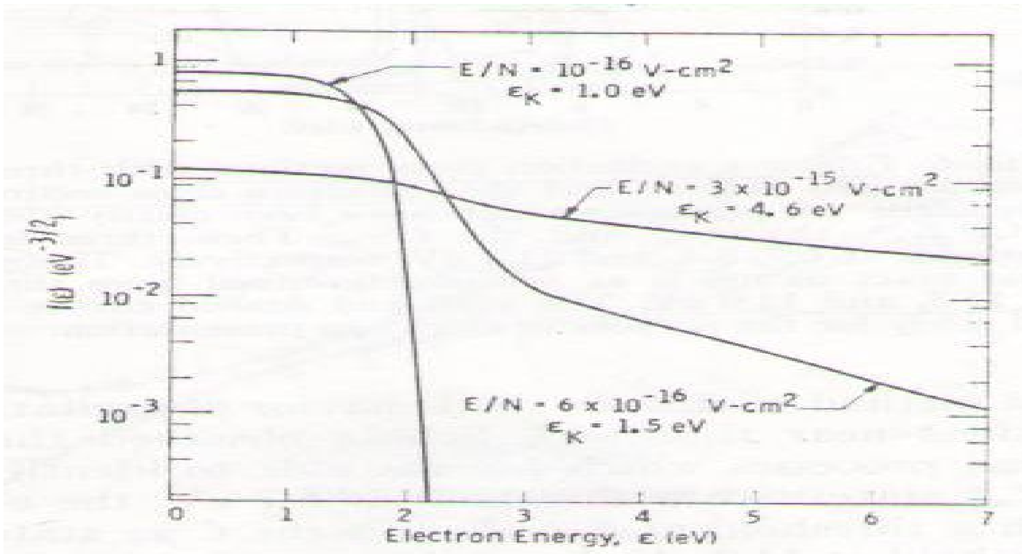
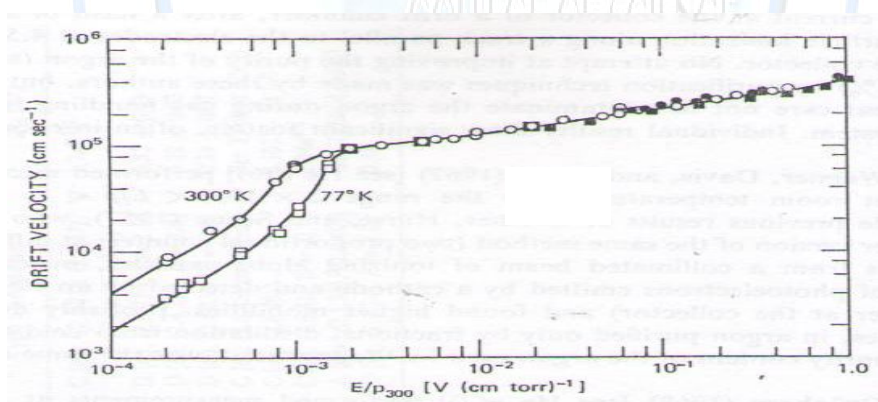
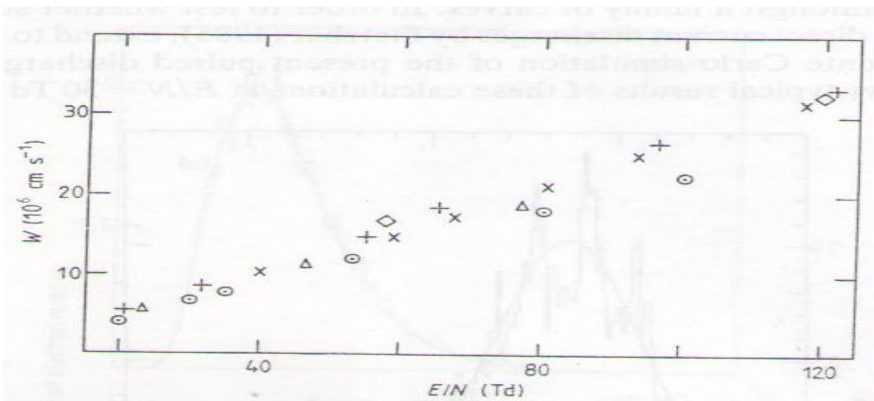


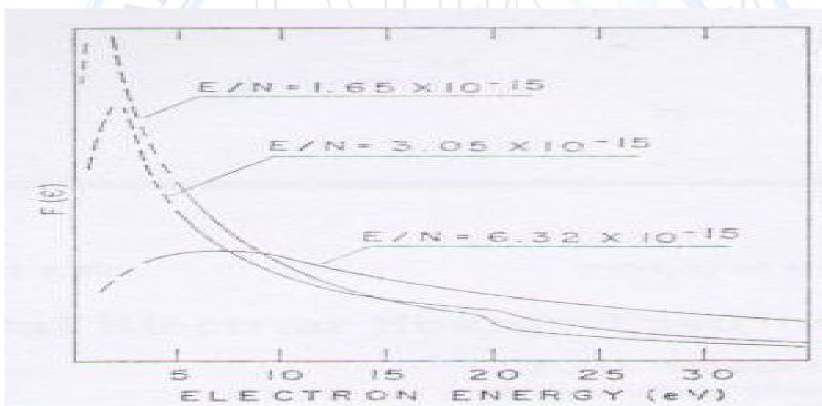
Fig.(5) : Energy distribution function f(ε) for electrons in N_2 for three values of E/N and corresponding values of eK, f(ε) is defined such that $\int_0^\infty \varepsilon^{1/2} f(\varepsilon)\, d\varepsilon = 1$.



Fig(6): ●Nielsen's [σ(1)], ■ Bowe's [σ(6)], and ○□ Pack's and Phelps's [σ(8)], experimental value of the drift velocity in argon, for $E/P<2\times10^{-4}$electrons are in thermal equilibrium with the gas; the corresponding μp_o values are 1.64and $4.0\times10^{7} cm^{2}V^{-1}$ torr, respectively, at 77 and 300^{0} K [after Pack and Phelps(1961)].



Fig(7): The electron drift velocity in helium as a function of E/N, ○ , represent data ; Δ, Anderson (1964); +, Phelps et al (1960), ×, Stern (1963): ◊, Kucukarpack et al (1981).



Fig(8): Experimental electron energy distributions for helium

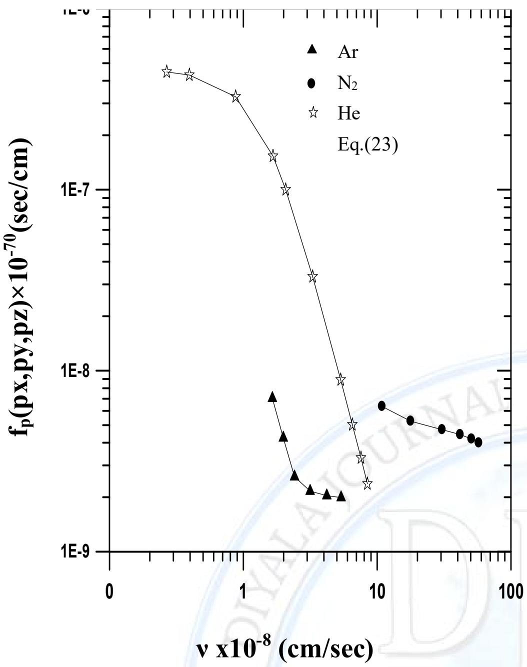


Fig.(9): The Probability density function f_p, versus the electron velocity ν, for Ar, He and N_2 gases.

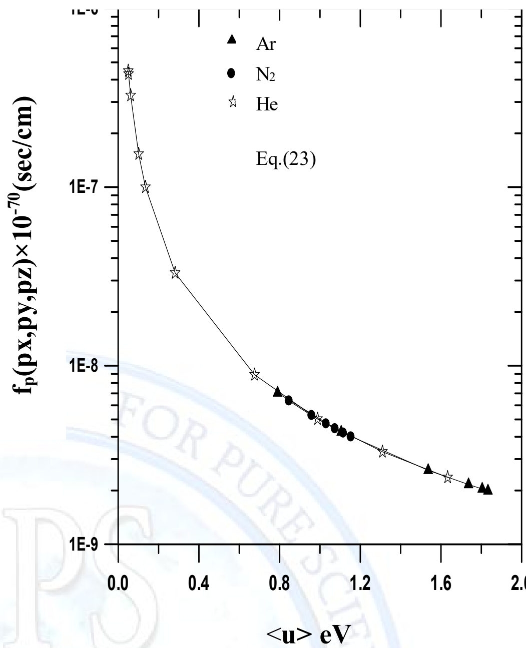


Fig.(10): The Probability density function f_p , versus the electron average energy <u> , for Ar, He, and N_2 gases.

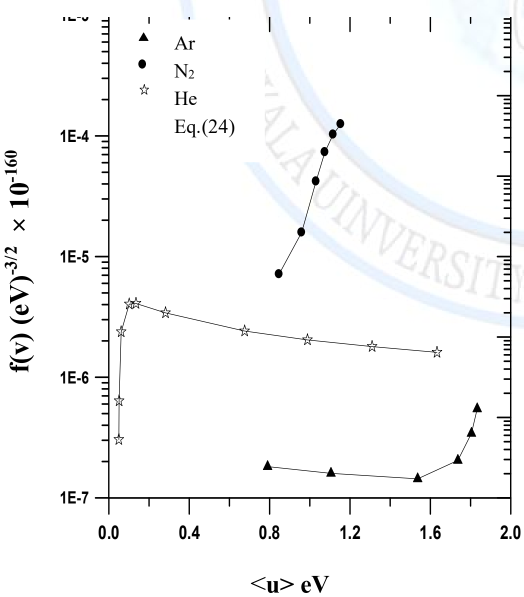


Fig.(11): The speed probability density functions of speeds f(ν) , versus the electron average energy,<u>, for Ar, He, and N_2 gases.

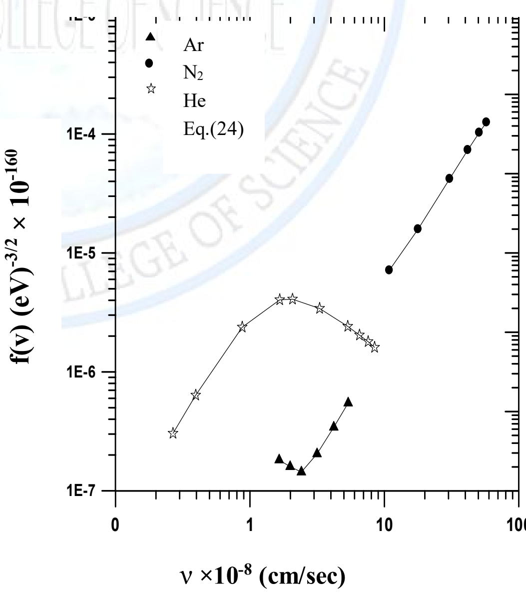


Fig.(12): The speed probability density functions of speeds f(ν), versus the electron velocity ν , for Ar, He, and N_2 gases.

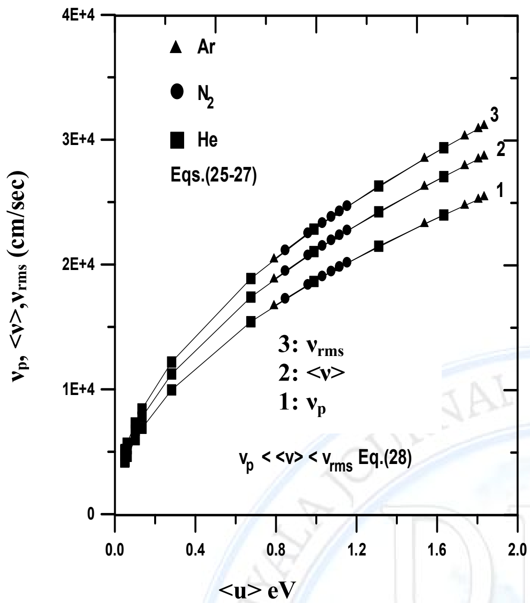


Fig.(13): The most probable speed ν_p , the mean speed ,<ν>, and the root mean square, ν_{rms}, as a functions of the electron average energy, <u>, for Ar, He, and N_2 gases.

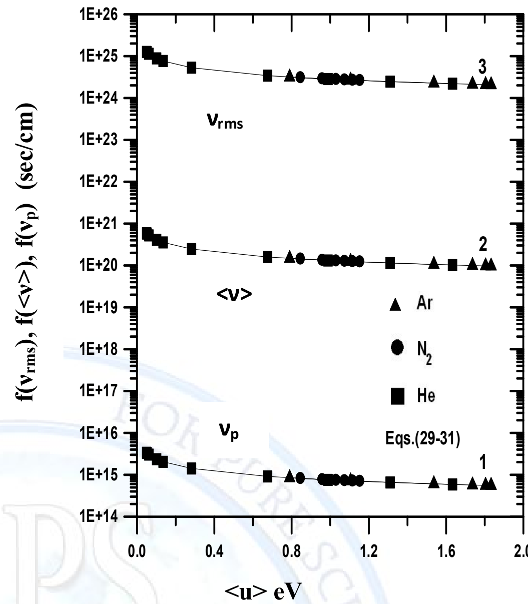


Fig.(14): The Maxwell-Boltzmann speed distribution probability versus the electron average energy ,<u>, for Ar, He, and N_2 gases.

References

1. Charles K. and Herbert K. (1980)Thermal Physics,2nd ed. (Freeman,Co.,New . York,)PP.87
2. Synge, J. L. (1957)The relativistic gas, Noord_Holland.
3. Vrhovac S.B., Stojanovic V.D., Jelenkovic B.M.,Petrovic Z.L.(2001)Electron distribution of Electrons in a Low-Current Self-Sustained Nitrogen Discharge, J. Appl. Phys., Vol.90, No.12,PP.5871-5877.
4. Tezcan,S.S.; Akcayol,M.A.; Ozerdem,O.C.; Dincer,M.C.;(2010), Calculation of Electron and Energy Distribution Functions From Electron Swarm Parameters Using Artificial Neural Network in SF6 and Argon, IEEE Transaction on Plasma Science,Vol.38, No.9, PP.2332-2339,Part 1.
5. Gilardini Aldo, (1972), Low Energy Collisions in Gases: Swarm and Plasma Methods Applied to Their Study. John Wiley , Sons New York, PP.74.

6. Dujko,S.;Ebert,V;White,R.D.;Petrovic,Z.L.;(2011), Boltzmann Equation Analysis of Electron Transport in a N-2-0-2 Streamer Discharge, Japanese J. Appl. Phys. Vol. 50, No. 8, PP.480-486.
7. Tkachev A. N. and Yakov lenko S. I., (2006), Electron Energy Distribution Function and Dense – Gas Ionization in the Presence of a Strong Field, Laser Physics. Vol. 16, No. 9, PP. 1308.
8. Hideaki Matsuura, et al., (2008), Distortion of Bulk – Electron Distribution Function and its Effect on Core Heating in Fast Ignition Plasmas, J. Physics: Conference Series, Vol. 112, PP. 1- 4.
9. Rockwood S. D. and Greene A. E., (1980), "Numerical Solution of the Boltzmann Equation, Computer Physics Communication, Vol. 19, pp. 377-393.
10. Won Young Yang, et al., (2005), Applied Numerical Methods Using Matlab, Wiley-Inters Science, A John Wiley, Sons, Inc, PP.290.
11. Matt Krems, (2007), The Boltzmann Transport Equation: Theory and Application, PP. 1-9.
12. Hoffman and Skarsgard , (1969) , Momentum Transfer Cross Section and Conductivity Ratios for Low _Energy Electrons in He, Ne, kr, and Xe, Phys. Rev., Vol. 178, No. 1, PP. 168-175.
13. Roberts T. D. and Burch D. S., (1966), Experimental Electron Energy Distributions for Townsend Discharges in Helium, Phys. Rev. Vol. 142, No.1, PP. 100-104.
14. Nikitovic,Z.;Radovanov,S.;Godet,L.;Raspopovic,Z.;Sasic,O.;Stajanovic,V.;Petrovic,Z.L.;(2011),Measurement and Modeling of Electron Energy Distribution in the Afterglow of a Pulsed Discharge in BF3,EPL,Vol.95,No.4,5981-5985.
15. Engelhardt A. G., Phelps A. V., and Risk C. G.(1961)Determination of Momentum Transfer and Inelastic Collision Cross Sections for Electrons in Nitrogen Using Transfer sport oefficients,Phy.Rev.,Vol.135, No.6A, PP.A1566-A1574.
16. Roberts T.D., and Burch D. S.(1966)Experimental Electron Distributions for Townsend Discharges in Helium, Phy.Rev.,Vol.142,No.1,PP.100-103.

17. Amies B. W., Fletcher J. and Sugawara(1985)Pulsed Electrical Discharges in Helium Gas, J. Phys. D: Appl. Phys. Vol.18,PP.2023-2028.

إيجاد احتمالية توزيع ماكسويل-بولتزمان لغازات النيتروجين(N_2)،الهليوم (^{4}He)والاركون(Ar^{40})

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الخلاصة

تم في هذا العمل بناء نموذج نظري لحساب توزيع ماكسويل-بولتزمان للغازات ،وأيضا حساب السرع النموذجية التي هي الأكثر احتمالا υ_p ، معدل السرعة $<\upsilon>$ ومعدل مربع الجذر للسرعة υ_{rms} ، إضافة إلى تحقيق شرط هذه السرع لغازات النتروجين، الاركون والهليوم عند درجة حرارة 300 درجة كلفن ; $[E/N=(0.5,1,2,3,4,5)\times10^{-16}$ $(1,2,4,6,8,10)\times10^{-18}$; (0.1214 , 0.182 , 0.455 , 1.214 , 1.82 , 4.55 , 12.14 , 18.2 , 24.3 , 30.3) $\times10^{-18}]$ ($V\ cm^2$) على التوالي .

عند مقارنة القيم التي حصلنا عليها باستخدام النموذج النظري مع النتائج العملية المنشورة لباحثين آخرين فأنها أظهرت تطابقا جيدا وان هذه القيم تم رسمها كدوال إزاء متغيراتها.

الكلمات المفتاحية: معادلة بولتزمن ، المقطع العرضي التصادمي، نقل الجسيمات المشحونة، معلمات الحشود.