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Theoretical Study of The Electron Energy Distribution Function in pure He and He- Cl_2 Gas Mixture

Research Project

Submitted to the department of Physics in partial fulfillment of the requirements for the degree of BSc. in Physics

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Erbil, KURDISTAN

April-2023

بِسْمِ ٱللَّهِ ٱلرَّحْمَٰنِ ٱلرَّحِيمِ

لَمَّا بَلَغَ أَشُدَّهُ آتَيْنَاهُ

حُكْماً وَعِلْماً

وَكَذَٰلِكَ نَجْزِي

الْمُحْسِنِينَ

سورة يوسف الآية 76

Supervisor Certificate

This research project has been written under my supervision and has been submitted for the award of the degree of BSc. in (Physics).

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Date 6 / 4 /2023

DECLARATION

I declare that the BSc. project entitled: **Theoretical study of the electron energy distribution function in pure He and He, chlorine gas mixture**. Is my own original work, and hereby certify that unless stated, all work contained within this thesis is my own independent research and has not been submitted for the award of any other degree at any institution, except where due acknowledgment is made in the text.

Student Name: Sima Kamal Aziz

Signature:

Date: 6/4/2023

Dedication

This thesis is dedicated to:

Allah Almighty, my Creator and my Master,

My great teacher and messenger, Mohammed (May Allah bless and grant him), who taught us the purpose of life,

My homeland Kurdistan, the warmest womb,

The University of Salahaddin-Erbil; my second magnificent home;

My great parents, who never stop giving of themselves in countless ways,

My beloved brothers and sisters;

To all my family, the symbol of love and giving,

My friends who encourage and support me, All the people in my life who touch my heart.

Acknowledgment

Firstly, and the most importantly, I would like to thank Allah the ultimate until the end day comes who have wonderful plans for me and have guided me to here at this moment. He has kept me strong and focused so that I would not go wrong.

I would like to express my sincere and deep appreciation to my supervisor: **Assist. Prof. Gulala Mohammed Faraj** for his constant encouragement, constructive suggestions and continuous discussion throughout the project. I am grateful to College of Education and the Department of Physics for supporting me during my study.I would like to extend my gratitude to the all of staffs and employs at Department of Physics, at collage of Education and at Salahaddin University-Erbil

Last and certainly not least, I would like to give my sincere thanks to all the members of my family for their love, continuous support, encouragement and understanding.

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Abbreviation

Abbreviation	Details
EEDF	Electron energy distribution Function
E	Applied electric field
m	Electron mass
T_e	Electron temperature
V	Electron velocity
∇_r	The special gradient in r- dimension
e/m	The ratio of electron charge to its mass which is refers to the acceleration due to applied electric field (E) ($V.cm^{-1}$).
∇_V	The velocity- gradient operator
E/N	Ratio of applied electrical Field to the total number density of molecules of gases
He	Helium gas
Cl_2	Chlorine gas

Summary

Plasma is described as an electrically neutral medium of unbound positive and negative particles. It is important to note that although they are unbound, these particles are not 'free'. When the charges move, they generate electric current with magnetic fields, and as a result, they are affected by each other's fields.

Theoretical calculations are performed on the electron energy distribution function (EEDF) in pure He and He-Cl_2 gas mixtures by using the two-term approximation of the distribution in Boltzmann equation within the international computer code **BOLSIC**

A set of electron cross-section data for each gas have been used in this calculation. The calculated distribution function found to be remarked non-Maxwellian that have energy variations and have longer tail.

From the present work, I found that adding Cl_2 gas to He gas effect weakly on the Electron Energy Distribution Function which reflected the import electron-molecule energy exchange processes

Finally, the main advantage of He-Cl_2 mixtures is to reach the ionization state of nitrogen atoms with less electron energy.

Chapter One

Introduction

Plasma is a special kind of ionized gas exists in many forms in nature and has a widespread use in science and technology. It and in general consists of: positively charged ions, electrons and neutrals (atoms, molecules). We call an ionized gas 'plasma' if it is quasi-neutral and its properties are dominated by electric and/or magnetic forces. (K. wiesemam;1996)

Or once can define plasma as an electrically neutral medium of unbound positive and negative particles .it is important to note that although they are unbound, these particles are note ‘free, when the charges move, they generate electric currents with magnetic fields, and as a result, they are affected by each other is field (Andrey.S;2015).

It is sometimes remarked that 95% (or 99%, depending on whom you are trying to impress) of the Universe consists of plasma. This statement has the double merit of being extremely flattering to plasma physics, and quite impossible to disprove (or verify). Nevertheless, it is worth pointing out the prevalence of the plasma state. In earlier epochs of the Universe, everything was plasma. In the present epoch, stars, nebulae, and even interstellar space, are filled with plasma. (Richard Fitzpatick;1998)

Plasmas are nowadays a well-established tool with a diverse field of technical applications. Beyond the already traditional usage for the purpose of lighting, as active media in lasers, for plasma cutting and welding, and as electrical conductor, new applications can be found like anisotropic etching, large scale plasma displays, or the field of surface modification in Industrial production. (Klaus Fesser, Dinklage, Soltwisch,2009).

Plasma is a distinct state of matter containing a significant number of electrically charged particles, a number sufficient to affect its electrical property and behavior, and plasma is often called the ‘‘fourth’’ state of matter. The study of energy distribution of electrons in weakly ionized gases has a long history and become increasingly important for the quantitative understanding of gas discharges plasma physics, laser physics, etc.

The electron energy distribution function f(E) is essential in plasma modeling because it is needed to compute reaction rates for electron collision reactions. (AbtisamA.Alakrout;2020) In this work we choose He and

Cl_2 as a sample to have our calculation and because the two are almost identical in molecular mass, equilibrium nuclear distance, dissociation energy and fundamental vibrational constants.

The momentum transfers cross- sections also alike (Kazunori.T….et al;2011). Helium is one of the noble gases in the periodic table. The helium element is an odorless, colorless, non-toxic, gas, it is less soluble in water and doesn't form chemical compounds essentially. The thermal conductivity and the caloric content of helium are exceptionally high. For helium metastable, diffusion is also taken into account.

Chlorine The name chlorine is derived from Chloris, meaning green, referring to the color of the gas. Chlorine gas is two- and one-half times as heavy as air, has an intensely disagreeable suffocating odor, and is exceedingly poisonous. In its liquid and solid form, it is a powerful oxidizing, bleaching, and disinfecting agent. The density of chlorine gas is approximately 2.5 times greater than air, which will cause it to initially remain near the ground in areas with little air movement. Chlorine is not flammable, but may react explosively or form explosive compounds with many common substances. (Including acetylene, ether, turpentine, ammonia, natural gas, hydrogen, and finely divided metals)

Chapter Two

The Distribution Function

The velocity distribution of electron in gases is of fundamental importance as in most discharges the current is mainly an electron deduce all the microscopic variables of physical interest for the species. One of the primary problems of kinetic theory consists in determining the form of the distribution function for a given system. The differential equation that governs the temporal and spatial variation of the distribution function under given considerations is known as the Boltzmann equation (Jordan.S and Ljubomir. A 1998).

The Types of Distribution Function

1- **Druyvesteyn Distribution**

In case where interaction particles are electrons, which interact with a gas in the presence of direct current electric filed, the system of electrons can be described by the Druyvesteyn distribution function**.** The Druyvesteyn Method offers the flexibility of being used, the first and second derivatives are calculated using the same process used in finding the plasma potential. therefore, a change of variables is necessary express the electron energy distribution with respect to the plasma potential. This makes the plasma potential the energy reference level. (Nicholas James Behlman;2009).

The Druyvesteyn distribution function drops off very faster at high kinetic, this means that there are few particles at high energy in a system which can be described by the Druyvesteyn distribution function.

2- **Maxwell -Boltzmann distribution**

The system, in which the motion of the particles is perfectly random, can be described by the Maxwell-Boltzmann distribution function because it is impossible to reach thermal equilibrium even at ideal case 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.

3-Boltzmann Distribution Function.

Is a powerful tool for analyzing transport phenomena within systems that involve density and temperature gradients. Consider a system with non-uniform particle density and temperature. In each place within the system there is a local range where the thermal velocities are given by an equilibrium distribution function. A non-equilibrium distribution function determines the probability of a particle within the system to be at some place and to have some thermal velocity.

The Boltzmann equation under a number of approximations that affect the solution. the main assumptions are that the interacting particles behave like hard spheres and the energy of the electrons is much greater that the thermal energy of the gas. (Gulala.M.F; 2002)

Types of Collision

1-Elastic collision

Collisions which when occur, no change takes place in the internal energy of the particles but only their kinetic energy gets redistributed. When electrons collide with gas molecules, between the collisions it is accelerated by the electric field. Since electrons are very light in weight, they transfer only a part of their kinetic the much heavier ions or gas energy to the molecules with which they collide. This results in very little loss of energy by the electrons and therefore electrons gain very high energies and travel at a much higher speed than the ions. Therefore, in all electrical discharge’s electrons play a leading role. So once can say only kinetic energy between the impinging electron and the target (atom or molecule) is exchanged, the internal state of the target remains unchanged (Othman, M , Taha, S.2020).

2- Inelastic Collision

Inelastic collisions, are those in which internal changes in energy take place within an atom or a molecule at the expense of the total kinetic energy of the colliding particle. The Collision Process in Gases often results in a change in the structure of the atom. Thus, all Collision Process in Gases that occur in practice are inelastic collisions. For example, ionization, attachment, excitation, recombination are inelastic collisions.

3- Superelastic Collision

Super elastic collisions are those in which the colliding particle does not lose its kinetic energy, instead gains some kinetic energy from the particle it is colliding with and accelerates at a faster rate after the collision.Most of the collisions in nature are inelastic collisions where the kinetic energy of the colliding object is converted into some other form of energy. Well, a super elastic collision occurs mostly in explosive reactions like nuclear fissions, reactors, supernovas, explosions, etc that create critical impact. This is a result due to a gain of the additional amount of kinetic energy without any loss of energy. (Mustafa k . Jssim, Enas A. Jawad and Jamal K. Alsaide .2019).

The Boltzmann Transport Equation

The behavior of the electron interaction with gas molecules is governed by the distribution in space, energy and time of electrons in the pure gas. The distribution function obeys a continuity equation which is known as the Boltzmann transport equation in the presence of an external electric field is (Shane .P…et al,2020):

$$\left(\frac{\partial}{\partial t} + \bar{v}\nabla_r + \frac{e\bar{E}}{m}.\nabla_v\right) f(\bar{x}, \bar{v}, t) = \frac{df}{dt} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots (1)$$

Where (f) is the electron velocity distribution function (EEDF), (V) the electron velocity, (∇_r) is the special gradient in r-dimension, while(e/m) is the ratio of electron charge to its mass which is refers to the acceleration due to applied electric field (E) ($V.cm^{-1}$) and (∇_V) is the velocity-gradient operator.The term on the right hand side of equation (1) is the collision integral, which accounts for electron energy transferred in elastic , inelastic collisions and super elastic collisions. (Gulala.M.F; 2002)

Chapter Three

Results and Discussion

Numerical Solution Method

Equation (1) was solved numerically by iteration method omitting the details of this method usually, while solving the Boltzmann equation numerically a uniform grid in energy space is used according to the experimental data (V. Yu. Bazhenov ….et al;2001) the effective electron temperature Te is 0.1eV, the pressure P=0.3 torr.In order to calculate the EEDF accurately, it is necessary to use a large number of grid points to make the energy interval Δu small with respect to Te .Helium gas is taken as a symbol to calculate the electron energy distribution function, after that we mixed Cl_2 gas with Helium (He) with different concentration.

Two types of cross sections are used for the analysis and these represent momentum transfer cross –section and ionization cross-sections these cross-section data are used as input data, therefore, eq (1) was solved numerically for a wide range of E/N values The E/N values were chosen to yield mean electron energies in the range (0.65-3.48) eV.

The calculate distribution functions in pure He is shown in fig (3.1) While fig (3.2) is representing the values of the electron energy distribution Function (EEDF)as a function of Electron energy values in He-Cl_2 gas mixtures with different concentration.

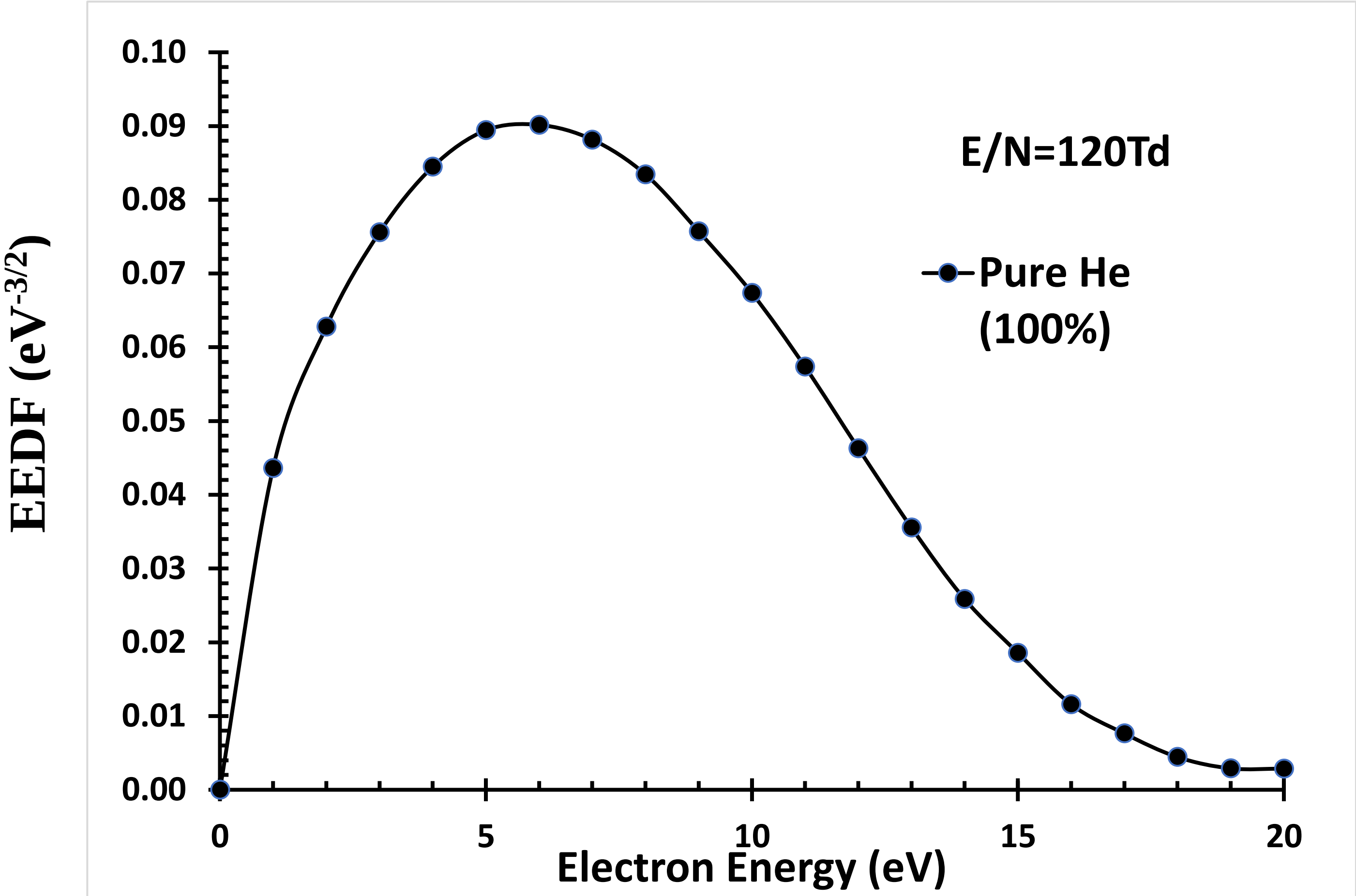

Figure (3.1): The Distribution Function as a Function of Electron Energy in pure He

Fig (1) represent the EEDF For pure (He) at E/N = 120Td as a Function of electron energy. In this Figure the Distribution is non- Maxwillian and had Longer tail equal to (20 ev)

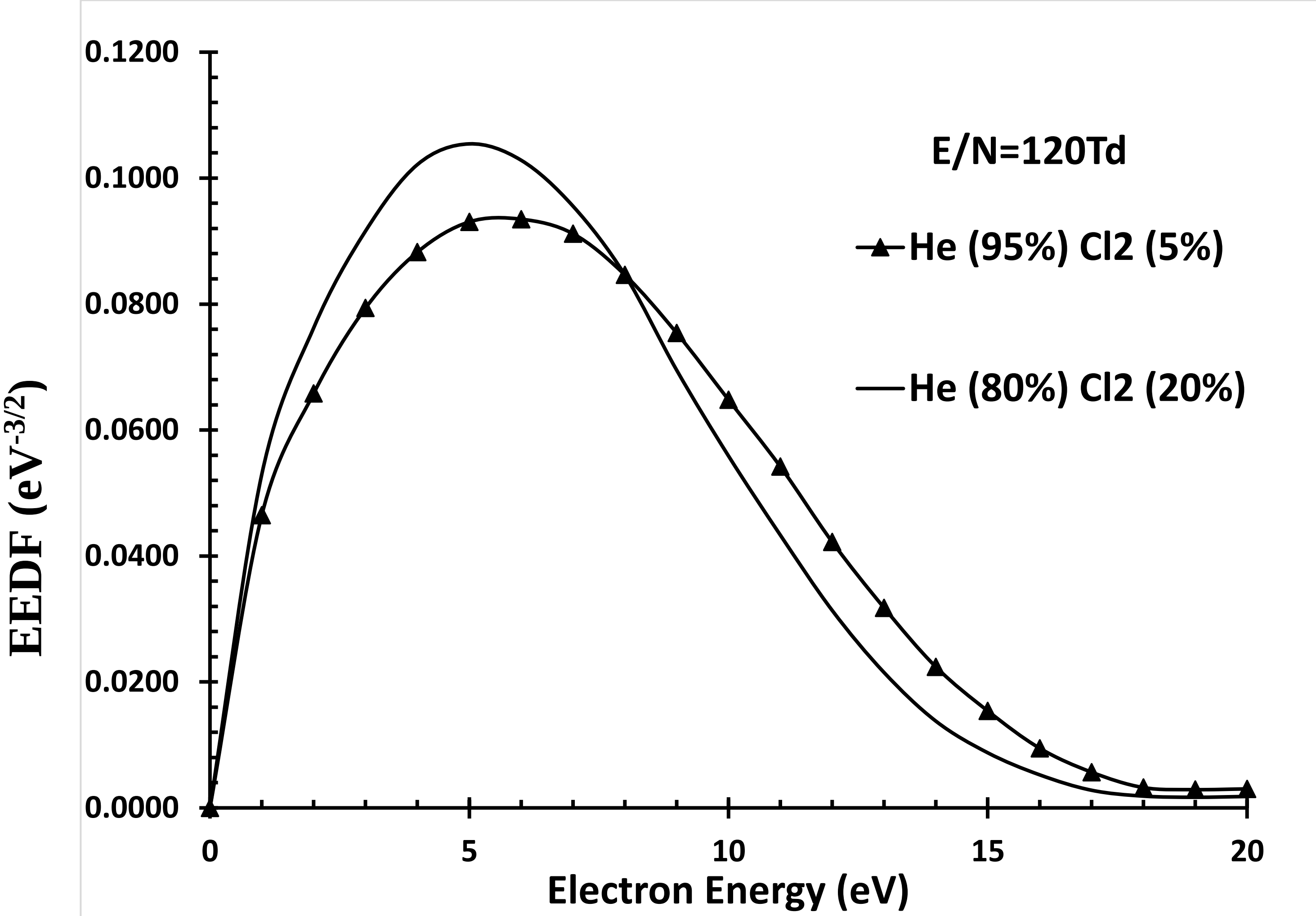

Figure (3.2): The Electron Energy Distribution as a Function of Electron Energy for (He-Cl_2) gas mixtures for different concentration.

In Fig (2) which is represent EEDF for (He-Cl_2) gas mixtures for different concentration, adding (5%) Cl_2 increase the distribution highest from 0.085ev for pure He to 0.90ev and to 0.1ev in case of adding (20%) cl_2 gas to He gas.

Actually, the change that can be seen in the highest of the Distribution Function is not too much and this is because of the accuracy of the calculations depends on the accuracy of electron-molecule cross-section's sets, also some of electron's have very weak energy and this increase the probability of attachment with neutrals atoms to create negative ions.

Chapter Four

Conclusion

By using the numerical **BOLSIG** code, it was possible to investigate the behavior of the Electron energy distribution function (EEDF) for pure Helium and Helium - Chlorine gas mixtures by using set of cross sections data for each gas.

Generally, it can be concluded from the present work that the EEDF is change by changing the concentration of each gas because this factor affected automatically on the electron energy distribution function highness, this means that the EEDF is increase by increasing the amount of Cl_2 in the mixture, On the other hand the calculated distribution function for He-Cl_2 gas mixtures is strongly depend on the parameter E/N, also because the electron acquired the enough energy from the applied electric field to reach the ionization level.

The main advantage of He-Cl_2 mixtures is to reach the ionization state of Helium atoms with less electron energy.

Finally, it can be interpreting that practically no one of the collision processes are neglected and also all the energy range are involved, Therefore, it needs to use different types of cross sections from many sets of published tables (as: electronic excitations, vibrations) In order to minimize the shift or the difference between the output values theoretically.

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