Salahaddin University-Erbil

Calculation of the Electron Energy Distribution and Ionization Coefficient in N_2-CO_2 gas Mixture Using Boltzmann Equation

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

By:
Asia Omer Ali

Supervised by:
Assist. Prof. Gulala Mohammed Faraj

Erbil, KURDISTAN

April– 2024

بِسْمِ ٱللَّهِ ٱلرَّحْمَٰنِ ٱلرَّحِيمِ

لَمَّا بَلَغَ أَشُدَّهُ أَتَيْنَاهُ

حُكْماً وَعِلْماً

وَكَذَٰلِكَ نَجْزِي

الْمُحْسِنِينَ

سورة يوسف **76**

DECLARATION

I declare that the BSc. project entitled**: Calculation of the Electron Energy Distribution and Ionization Coefficient in N_2-CO_2 gas Mixture Using Boltzmann Equation**. 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.

Signature:

Student Name: Asia Omer Ali

Date: April-2024

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.

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 swarm parameter (i.e Ionization coefficient) and electron energy distribution function (EEDF) in N_2/CO_2 gas mixtures by using the two-term approximation of the distribution in Boltzmann equation within the international computer code Boltz.

A set of electron cross-section data have been used in this calculation.

TABLE OF CONTENTS

LIST OF FIGURES

ABBREVIATIONS

Abbreviation	Details
α/N	Ionization Coefficient
σ_i	Ionization Cross Section
N	Total number density
F(u)	Distribution Function
σm	Momentum transfer cross-section
K	Boltzmann Constant
T	Temperature
δf /δt	Rate of change of Distribution Function
EEDF	Electron energy distribution function
CFDL	Current-free double layer
V	Electron velocity
E	Electric field
∇_v	Velocity-gradient
∇_r	Special gradient in r-dimension
t	Time
ε	The electron mean energy
$d\varepsilon$	mean Energy loss
eV	Electron volt
P	pressure
V_d	Drift Velocity
m	Electron mass
E/N	Ratio of applied electrical field to the total number density of molecules of gases

Chapter One

Introduction

A plasma, the so-called 4th physical condition of matter, is defined as a (partly) ionized gas, which is neutral in average ("quasimetric") and exhibits collective properties (the density has to be high enough. Thus, the plasma consists in most cases of neutral atoms or molecules, positive ions and electrons, which interact by collisions, for this purpose, a fraction of the electrons has to have kinetic energies which exceed the ionization potential, i.e. above a few eV, so that the electrons have to be rather "hot

The study of energy distribution of electrons in weakly ionized gases has a long history that goes back to 1960s and become increasingly important for the quantitative understanding of gas discharges plasma physics, laser physics…etc.

Electron energy distribution functions in low degree ionized gases are of fundamental importance in understanding ionization phenomena in gases and provide a link between theory and measurements.

A Boltzmann approximation analysis for electron in nitrogen and carbon dioxide under an electric field will be intends theoretically for determination of the electron collision cross-section. (Schekochihin, A. A. 2022)

The role of electron swarm parameter (i.e ionization coefficient which is the mean number of ionizations per cm in the field direction produced by electron collision) is an important one because it provides a link between electron-gas collision cross-section and gas breakdown discharge phenomena.

N_2 and CO_2 are important component gases of the CO_2laser, which is one of the most efficient gas lasers. The two are almost identical in molecular mass, equilibrium nuclear distance, dissociation

energy and fundamental vibrational constant. The momentum transfer cross-section is also alike. (Sh.Kh.Al-Hakary,2016)

Nitrogen is a colorless, odorless, and tasteless gas, it is slightly lighter than air. Also, it is a non-poisonous gas but animals die due to suffocation of nitrogen.

The most important chemical property of this gas is that it is non-combustible gas neither does it support burning and chemically inert under ordinary conditions.

Carbon dioxide is a chemical compound composed of one carbon and two oxygen atoms bonded together. It is a colorless and odorless gas; it is a non-flammable gas and it is slightly toxic and denser than air. Also, its solubility decreases as temperature increases. (Jebur, K. S…*etal*. 2019)

Chapter Two

Theory

In plasma physics, distribution functions describe the statistical properties of charged particles within a plasma. These distribution functions provide information about the velocity, energy, and spatial distribution of the particles in the plasma.

There are several distribution functions commonly used in plasma physics, three crucial distribution functions are Maxwell, Boltzmann, and Maxwell-Boltzmann, each playing a significant role in understanding the behavior of particles in gases and thermal equilibrium. (Gulala. M.F, 2002)

1-Maxwell Distribution Function

The Maxwell distribution function, named after the renowned physicist James Clerk Maxwell, addresses the probability distribution of particle speeds in a gas at a specific temperature. Maxwell made significant contributions to our understanding of kinetic theory and ideal gases. His work culminated in the development of the Maxwell distribution function, which is essential for describing the statistical properties of particles in gases. This function is characterized by its bell-shaped curve, with the peak corresponding to the most probable speed at a given temperature.

Applications:

The Maxwell distribution function finds widespread application in various fields, including gas dynamics, statistical thermodynamics, and astrophysics. It aids in understanding the distribution of speeds and kinetic energies of gas molecules. (Godyak, V…. *etal.* 2002)

2- Boltzmann Distribution Function

Ludwig Boltzmann, a pioneering figure in statistical mechanics, introduced the Boltzmann distribution function. This function describes the probability distribution of particles over different energy levels within a system at a specific temperature.

Boltzmann's work laid the foundation for the statistical interpretation of entropy and thermodynamics, linking the microscopic behavior of particles to macroscopic thermodynamic properties.

Applications:

The Boltzmann distribution function is of paramount importance in statistical mechanics and quantum physics. It allows scientists and engineers to analyze the occupation of energy states in various systems, from ideal gases to condensed matter and quantum systems. It is a cornerstone in the study of statistical ensembles and serves as the basis for understanding the relationship between microscopic and macroscopic properties. (Encarnaçao, P. M…*etal* ,2016)

3- Maxwell-Boltzmann Distribution Function

The Maxwell-Boltzmann distribution function amalgamates aspects of both Maxwell and Boltzmann's work. It describes the statistical distribution of speeds for particles in a gas, accounting for both the kinetic energy (as in the Maxwell distribution) and the distribution of particles over energy levels (as in the Boltzmann distribution). This combined approach provides a comprehensive view of the statistical behavior of gas particles.

Applications:

The Maxwell-Boltzmann distribution function is of particular importance in fields like statistical thermodynamics, chemistry, and plasma physics. It enables the modeling of gas particles in a more complete manner, considering both their speed distribution and energy state occupation. This function is indispensable for understanding gas properties and behavior in a wide range of physical systems. (Boenig. H, 2019).

4- Druyvesteyn Distribution Function

The Druyvesteyn distribution function is a way to describe the electron energy distribution function (EEDF) in plasmas.

It is an extension of the Langmuir and Mott-Smith probe theory that allows the determination of the electron energy spectrum.

The Druyvesteyn formula is used to fit the EEDF data.

The Druyvesteyn-like distribution tends to a Maxwellian distribution and it is used to describe the bounded plasma, and the complex permittivity for the plasma with Druyvesteyn distribution is calculated. The Druyvesteyn theory is also used to study the electron energy distributions upstream of a current-free double layer (CFDL) contained. (Godyak, V. A…*etal*, 2002)

.

Collision

Collisions occur when one object strikes another. Problems involving collisions are usually solved using conservation of momentum and conservation of energy.

Types of Collisions:

Collisions are fundamental events in physics, and they play a crucial role in understanding the behavior of particles and systems in various physical contexts. In this section we will discuss different types of collisions in classical physics and then explore how these concepts apply to the field of plasma physics, where collisions have unique characteristics and significance.

In classical physics, there are three main types of collisions based on how momentum and kinetic energy are conserved during the collision:

1-Elastic Collisions:

In an elastic collision, both momentum and kinetic energy are conserved. The total kinetic energy of the system before the collision is equal to the total kinetic energy after the collision.

The objects involved rebound off each other without any loss of energy.

Examples include collisions of billiard balls, ideal gas molecules, and objects on a frictionless surface. (Fayyadh, I. K. ..*etal*,2020)

2-Inelastic Collisions:

In an inelastic collision, momentum is conserved, but kinetic energy is not conserved. Some of the initial kinetic energy is transformed into other forms of energy during the collision, such as internal energy or work done.

The objects involved typically stick together or deform during the collision.

Examples include car collisions, where kinetic energy is converted into thermal energy and deformation energy.

3- Super Elastic collision

Super elastic collision is a collision in which potential energy is converted into kinetic energy so that the total kinetic energy of the colliding objects after collision is greater after the kinetic energy before collision, for example an Explosion. (Jawad, E. A ,2018)

Boltzmann Transport equation

The behavior of electron interaction with gas molecules is governed by the distribution in space, energy and time of electrons in the pure gas or in a mixture of gases. The distribution function obeys a continuity equation which is known as the Boltzmann transport equation.

The general form of the Boltzmann equation is (W.L. Morgan, 1995):-

$$\left(\frac{\partial}{\partial t} + V.\nabla r - \frac{eE}{m}.\nabla_V\right) f\left(r, v, t\right) = \left(\frac{\delta}{\delta t}\right)_{coll.} \quad \text{..........................(1)}$$

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 and inelastic collisions.

It is well known that the swarm parameters of electrons and collision cross-sections with molecules are related to each other through the medium of the velocity distribution function of the swarm. Therefore, the ionization coefficient can be calculated from. (Gulala. F, 2002).

Transport parameter

Electron-transport parameters in gases have long been studied and proved to be indispensable in determining appropriate cross sections of elastic and inelastic collisions between gases and slow electrons and the most transport parameter is the ionization coefficient.

Ionization coefficient

The electron ionization coefficient α is importance in all cases where an electric field E and thus a mean electron energy ε for a specific energy distribution is given, so that the rate of ionization per colliding electron per second (W.L. Morgan; 1995): -

$$\frac{\alpha}{N} = \frac{1}{V_d}\left(\frac{2e}{m}\right)^{1/2}\int_0^\infty \sigma_i(\varepsilon)\, f(\varepsilon)\, d\varepsilon \ldots\ldots\ldots\ldots\ldots\ldots \quad (2)$$

Where ($\frac{\alpha}{N}$)is the ionization coefficient of electron and (V_d) is the drift velocity, (m) is the electron mass and $\sigma_i(\varepsilon)$ is the ionization cross-section. (Othman, M. M., & Hussein, S. R, 2020)

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 0.3eV, the pressure P-0.2 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

Mixtures of Nitrogen and Carbon dioxide gas is taken as a symbol to calculate the Electron Energy Distribution Function with two different concentrations.

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 (0.65-3.5) eV.

The calculate distribution functions in N_2-CO_2, gas mixtures are shown in fig (3.I) While fig (3.2) is representing the values the ionization coefficient as a function of E/N values in N_2-CO_2 gas mixtures with two different concentrations.

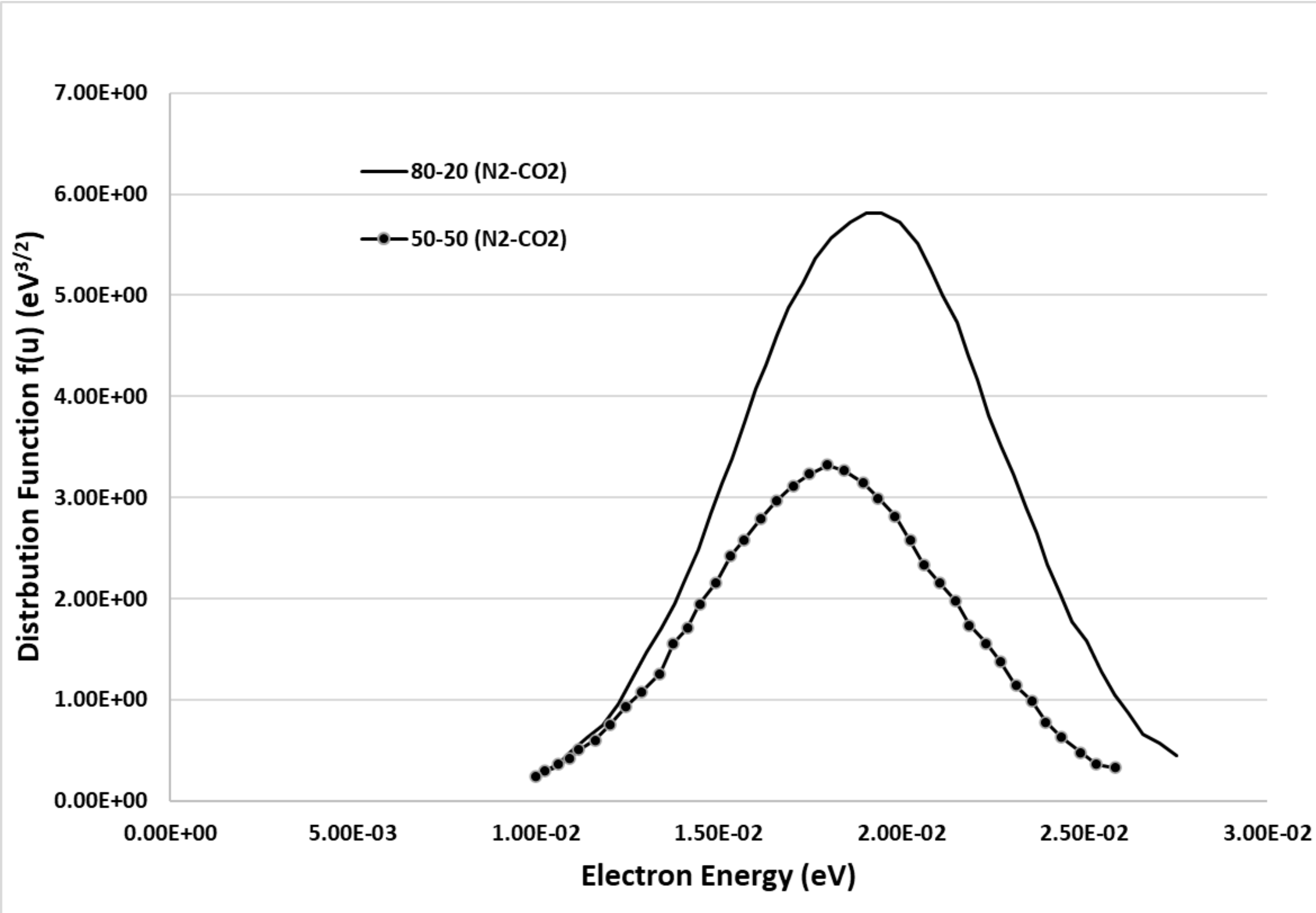
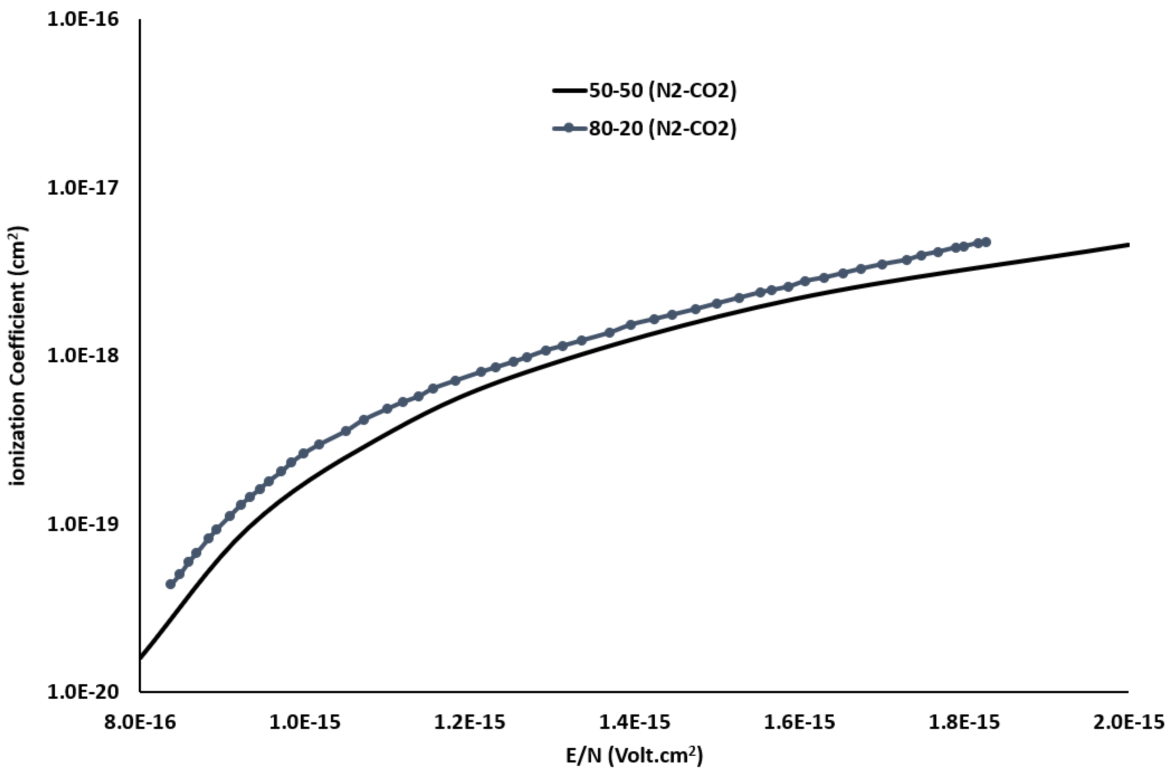


Fig (3.1): The Distribution Function as a function Electron Energy in N_2- CO_2 gas mixtures for two different concentrations.

In fig (3.1); which is represent the Electron Energy Distribution Function for N_2-CO_2 gas mixtures as a Function of electron energy at E/N=27 Td [where E is the electric Field to the gas Density].

It can be note that the EEDF For (80-20: N_2-CO_2) gas concentrations had grater highest than the concentration (50-50: N_2-CO_2), This is mean that the distribution Function is affect strongly by the concentration of each gas in our mixtures, this attributed to the electron collision number's.



Fig(3.2): The ionization coefficient as a function of E/N values for N_2-CO_2 gas mixtures for two different concentrations.

Fig (3.2) is representing the ionization coefficient as a function of E/N value for N_2-CO_2 gas mixture with two different concentration which is calculated using eq (2).

This figure shows its behavior which is nonlinear with increase of E/N

because the electrons acquire enough energy from the applied electric field So the number of energetic electronic which cause the ionization, increase with increasing E/N according to the ionization cross-section.

Chapter Four

Conclusion

By using the numerical Boltz code, it was possible to investigate the behavior of the Electron energy distribution function for N_2-CO_2 gas mixtures by using set of cross sections data, the calculated distribution function is found to be remark non-Maxwellian.

The process of ionization is causing an increase in E/N value, this means that the electron acquired the enough energy from the applied electric field to reach the ionization level.

The EEDF is strongly depend on the concentration of each gas in the mixtures.

Generally, it can be concluded from the present work that any change in the gas concentration value will cause a serious variation in related transport parameters which can be attributed to the activities of electron interactions with the medium constituents.

Finally, it can be interpreted 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.

References:-

Agrafonov. Y. & Petrushin, I. (2015). Two-particle distribution function of a non-ideal molecular system near a hard surface. Physics Procedia, 71, 364-368.

Bazhenov, V. Yu & RrabtSev, A.V.2001.Investigition of the electron energy distribution function in hollow –cathode Glow Discharges in Nitrogen and Oxygen. Plasma physics report. Vol.27, No. 9, pp (813-818).

Boenig, H. (2019). Plasma science and technology. Cornell University Press.

Cadogan, S. P., Maitland, G. C., & Trusler, J. M. (2014). Diffusion coefficients of CO2 and N2 in water at temperatures between 298.15 K and 423.15 K at pressures up to 45 MPa. Journal of Chemical & Engineering Data, 59(2), 519-525.

Chiad, B. T. (2010). Study of electron energy distribution function and transport parameters for CF4 and Ar gases discharge by using the solution of Boltzmann equation-Part I. Iraqi Journal of Physics, 8(13), 1-9.

Encarnaçao, P. M., Cortez, A. F., Veenhof, R., Neves, P. N. B., Santos, F. P., Trindade, A. M. F., ... & Conde, C. A. N. (2016). Experimental Ion Mobility measurements in Ne-CO2 and CO2-N2 mixtures. Journal of Instrumentation, 11(05), P05005.

Fayyadh, I. K., Oufi, A. M., Alwan, A. I., & Abdulhasan, J. A. (2020, April). Effect of gas concentration on the electron transport and the plasma parameters of the CO2 gas mixture. In Journal of Physics: Conference Series (Vol. 1484, No. 1, p. 012022). IOP Publishing.

Fayyadh, I. K., Saud, N., Alaboudi, J. A., Alwan, A. I., Kadhim, R. O., & Hasan, N. M. (2020, November). Swarm of Electron Simulation in Carbon Dioxide Parameters for Intermediate E/N Values. In IOP Conference Series: Materials Science and Engineering (Vol. 928, No. 7, p. 072083). IOP Publishing.

Gulala.M.F .2000. Theoretical analysis of the electron energy distribution function in a weekly ionized gas using Boltzmann equation, M.Sc. Thesis, University of Salahaddin- Erbil.

Galaly, A. R., & Dawood, N. (2022). Theoretical and Experimental Study of the Effect of Plasma Characteristics on the Mechanical Properties of Ihram Cotton Fabric. Membranes, 12(9), 879.

Godyak, V. A., Piejak, R. B., & Alexandrovich, B. M. (2002). Electron energy distribution function measurements and plasma parameters in inductively coupled argon plasma. Plasma Sources Science and Technology, 11(4), 525.

Jawad, E. A. (2018, May). Theoretical Calculation of the Electron Transport Parameters and Energy Distribution Function for CF3I with noble gases mixtures using Monte Carlo simulation program. In Journal of Physics: Conference Series (Vol. 1003, No. 1, p. 012089). IOP Publishing.

Jebur, K. S., Jassim, M., & Jawad, E. A. (2019, July). Study the effect of addition of Ar to N2 gas on the EEDF and the correspondent coefficients of electron transport. In AIP Conference Proceedings (Vol. 2123, No. 1). AIP Publishing.

Lieberman, M. A., & Lichtenberg, A. J. (1994). Principles of plasma discharges and materials processing. MRS Bulletin, 30(12), 899-901.

Othman, M. M., & Hussein, S. R. (2020). Boltzmann equation studies on electron swarm parameters for oxygen plasma by using electron collision cross–sections. Zanco Journal of Pure and Applied Sciences, 32(5).

Schekochihin, A. A. (2022). Lectures on kinetic theory and magnetohy drodynamics of plasmas. Lecture Notes for the Oxford MMathPhys Programme.

Sh.Kh.Al-Hakary,2016, effect of pressure and hot filament cathode on some plasma parameters of hollow and argon glow discharge plasma, modern physics.

شیكردنەوەی نەخشەی دابەشبوونی ووزەی ئەلكترۆن و هاوكولكه ی به ئایون بوونی تیكه له ی گازی N_2-CO_2 به به كار هینانی یاسای بۆلتزمان

تێزیكە

پێشكەشی ئەنجومەنی كۆلێژی پەروەردە كراوە لە زانكۆی سەلاحەدین-هەولێر
وەكو بەشێك لە پێداویستیەكانی بەدەستهێنانی پلەی بەكالۆریۆس لە فیزیك

لە لایەن
ئاسیا عمرعلي

بە سەرپەرشتی
پ.ی.م. گوڵاڵە محمد فرج

نیسان 2024