

Transport coefficients calculation using Inference the Momentum-Transfer and Inelastic-Collision Cross Sections of Electrons in Carbon Dioxide

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Abstract

In this work, we were calculate the electron diffusion coefficients, such as, the drift velocity, characteristic energy, and collision frequencies using the cross sections of the momentum transfer and inelastic for electrons in CO₂ from figure(1) after solving the Boltzmann transport equation numerically using the Finite-Difference Method in gas medium through applied electric field at 300 °K.

The theoretical predictions were obtained in agreement with the experimental values was published.

Keywords: CO₂ lasers, Boltzmann Transport Equation, RF Discharges, Transport coefficients, Plasma discharge, Drift velocity.

الخلاصة

في هذا العمل ، تم حساب معاملات انتشار الالكترونات مثل سرعة الانجراف، الطاقة المميزة و ترددات التصادم باستعمال المقاطع العرضية المرنة وغير مرنة للالكترونات في غاز ثاني أوكسيد الكربون CO₂ من شكل (1) خلال حل معادلة الانتقال لبولتزمان عددياً باستخدام طريقة التفريق المحدد في وسط غازي بعد تسليط مجال كهربائي عليه عند درجة حرارة 300 كلفن . النتائج التي تم الحصول عليها تنبأ بأنها متوافقة مع النتائج العملية المنشورة.

Introduction

The determinations of momentum transfer and inelastic cross sections for electrons in CO₂ from experimentally measured values of transport coefficients.

The analyses were most accurate for the calculation of the cross sections for momentum-transfer and vibrational excitation, in addition the electronic excitation in CO₂. These results were an extension of previous calculations of cross sections in Hydrogen [1], [2], and [3], Deuterium [2], Nitrogen [1],[4], and the rare gases [5].The time-and space-independent Boltzmann transport equation were solved for distribution function of electron energies \mathcal{E} in a neutral gas using an initial set of elastic and inelastic cross sections. The calculations of the transport coefficients were done by taking averages [1], [2], [6], and

[7] over this distribution function and were compared with experimental values of the same transport coefficients. When the calculated values were match the experimental values to within 5% over an extended range of the ratio of the electric field strength E to gas density N, the cross section were considered satisfactory [8].

Carbon Dioxide

The very large energy exchange frequency at very low characteristic energy \mathcal{E}_k , and availability the \mathcal{E}_k and the recent time-of-flight drift velocity; these leading were to undertake on an analysis of the coefficient data of the electron transport in CO₂. Because of the CO₂ lasers development, the interest in excitation

cross sections for electrons in CO₂ was increased.

Boltzmann transport equation:

The electrons swarms were undertaken the applied electric field considering the steady state f^o distribution as [9][10]:

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

whereas G represents the energy loss factor, v represents the electron velocity, v_m represents the momentum transfer collision frequency; °T_g represents the gas temperature, K represents the Boltzmann factor. e represents the electron charge, and E represents the electric strength along the negative Z - axis direction.

Solution of transport equation:

After we were preparation the cross sections for vibration excitation, electronical excitation, ionization and momentum transfer in CO₂ would be feeding to the computer program [11]. Hence solves the Boltzmann transport equation numerically.

Determination of transport parameters:

The transport coefficients v_d, D/μ, v_m and v_u were obtained by solving the transport equation numerically (1) as above according to:

(a): the momentum transfer collision frequency v_m which was defined by [12][13]:

$$\frac{v_m}{N} = \frac{e E}{m N} \frac{1}{V_d} \dots\dots\dots (2)$$

this parameter v_m was primarily sensitive to the cross section for momentum transfer.

(b): the energy exchange collision frequency v_u which was defined by:

$$\frac{v_u}{N} = \frac{e V_d}{N} \frac{E/N}{\epsilon_k - kT} \dots\dots\dots (3)$$

this parameter v_u was primarily sensitive to the inelastic cross section.

(c): the drift velocity v_d, defined by [14][15]:

$$v_d = \mu E \dots\dots\dots (4)$$

$$\mu = -\frac{1}{3} \left(\frac{2e}{m} \right)^{1/2} \frac{\int_0^\infty \frac{u}{\sum_k N_k Q_m^k(u)} \frac{df^o}{du} du \dots\dots\dots (5)$$

$$(d): \epsilon_k = e \frac{D}{\mu} \dots\dots\dots (6)$$

where, e represents the electron charge 1.6×10⁻¹⁹ coulomb, m represents the electron mass, 9.109×10⁻²⁸ gm, E represents the applied electric field, V/cm, N represents the gas number density cm⁻³, v_d represents the drift velocity, cm/sec, ε_k represents the characteristic energy (eV), K represents the Boltzmann constant, 1.3805×10⁻²³ j/°k, °T_g represents the gas temperature in unit of Kelvin (°K), μ represents the mobility of electron (cm² sec⁻¹ V⁻¹), u represents the electron energy (eV), N_k represents the total number density cm⁻³, Q_m^k(u) represents the momentum transfer cross section (cm²) for elastic collisions of electrons of energy u(eV), D/μ represents the ratio of the diffusion coefficient to the mobility (eV).

Results and Discussion:

The electron transport coefficients were analyzed used in terms of elastic and inelastic cross sections as presented in Figure 1 [16], which was showing that many interesting conclusions can be reached regarding the magnitude and energy dependence of the cross sections.

Figure 1 represents the cross sections for momentum transfer Q_m, vibrational excitation Q_v, electronic excitation Q_x and ionization Q_i [16].

The curves were show the cross sections derived in your analyses of the data of Figure 4 and have a resonance nature with energy losses and the thresholds at 0.3, 0.6 and 0.9 eV and high energy tail of the 0.3 eV process. The magnitudes of these cross sections, the magnitudes of the resonance portion of the 0.083 eV energy loss process and the Q_m(ε) curve were adjusted to give a good fit to v_m and v_u curves calculated from the 300 °K data.

Figure 2 was show the drift velocity of the electron as a function of the applied electric field to the gas number density ratio E/N , which was increased proportionally with E/N and appeared agreement with experimental data [16].

Figure 3 appeared the characteristic energy was stable between $(2 \times 10^{-19} < E/N < 2 \times 10^{-17}) \text{ V cm}^2$ but proportionally increasing with E/N . These data was agreement with experiment values [16]. From Figure 4 was note that the our procedure of fitting to the v_m and v_u curves leads to rather satisfactory agreement between the calculated and experimental v_d , and D/μ values show in Figures 2 and 3, further experimental and theoretical investigations of this E/N range are necessary in order to resolve this discrepancy.

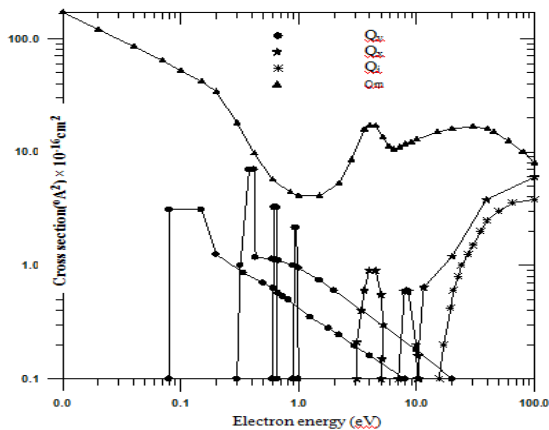


Figure 1: The inelastic scattering Q_v , Q_x , Q_i and momentum transfer Q_m cross sections versus the electron energy in Co_2 [17].

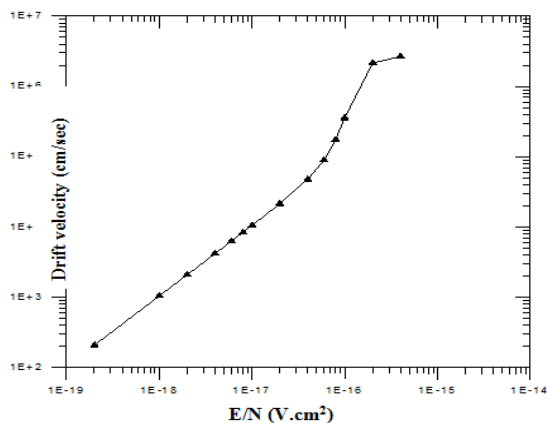


Figure 2: The drift velocity V_d of the electrons versus the applied electric field to the gas number density ratio, E/N in Co_2 .

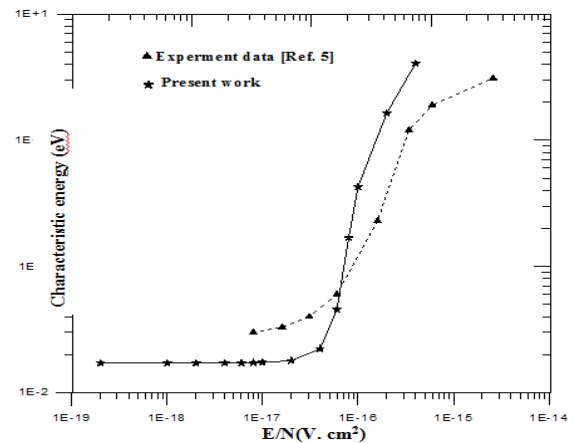


Figure 3: The characteristic energy D/μ of the electrons versus the applied electric field to the gas number density ratio, E/N in Co_2 .

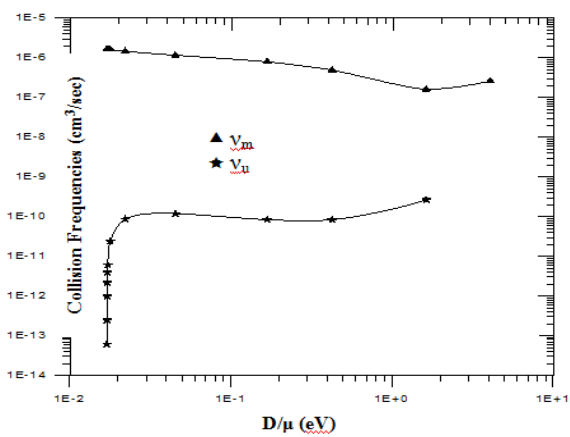


Figure 4 :The momentum transfer V_m and energy-exchange V_u collision Frequencies per molecule versus the characteristic energy, D/μ for electrons in Co_2 at 300ok.

Conclusions

The high quality experimental electron transport coefficient data was worthwhile. From the above the various gases and gas temperatures were to fill in the many gaps and check the questionable data evident. Such data were available for gases such as CO_2 , H_2O and CH_4 over a wide range of E/N values.

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