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ELECTRON TRANSPORT DATA IN N_2-O_2 STREAMER PLASMA DISCHARGES

SAŠA DUJKO[1,2], UTE EBERT[2], RONALD WHITE[3]
and ZORAN Lj. PETROVIĆ[1]
[1]*Institute of Physics, University of Belgrade, P.O.Box 68,*
11080 Zemun Belgrade, Serbia
E-mail: sasa.dujko@ipb.ac.rs
[2]*Centre for Mathematics and Informatics (CWI), P.O.Box 94079,*
1090 GB Amsterdam, The Netherlands
[3]*ARC Centre for Antimatter-Matter Studies, School of Engineering and Physical Sciences, James Cook University, Townsville 4810, Australia*

Abstract. A multi-term theory for solving the Boltzmann equation and a Monte Carlo simulation technique are used to investigate the electron transport in mixtures of molecular nitrogen and oxygen. We investigate the way in which the transport coefficients and spatially resolved transport data are influenced by the amount of O_2 in the mixture. This study was initiated in order to obtain the transport data for input into the fluid models and fluid components of hybrid models of streamers and has resulted in a database of such transport data.

1. INTRODUCTION

Streamers are growing filaments of weakly-ionized non-stationary plasma produced by an ionization front that moves through the non-ionized matter (Ebert et al. 2006). They have applications in diverse areas of science and technology ranging from their role in creating the lighting and transient luminous events in the upper atmosphere (Ebert and Sentman 2008) to industrial applications such as those used for the treatment of the polluted gases and water (Grabowski et al. 2005) and those employed for the plasma enhanced vapor deposition in microelectronics (Babayan et al. 1998). There have been numerous simulations of streamers (see, e.g. Ebert et al. 2006 and references therein), but the recent 3-dimensional self-consistent hybrid model of Li et al. 2009, is of special interest. In this model, the fast non-equilibrium electrons in the leading part of the ionization front are treated by a Monte Carlo simulation while the low-energy electrons in the rest of the domain are treated using a fluid model. The fluid part is based on the local field approximation and requires the tabulation of electron transport coefficients as a function of the reduced electric field. The fluid model is coupled with the Monte Carlo model via a model interface. To ensure the stable and correct interaction

between these two models, the correct implementation of swarm transport data and accuracy of their calculations are critical steps in modeling. Moreover, in this work we try to show which aspect of kinetic theory developed for swarm physics and which segments of data would be important for further improvement of both fluid and hybrid models of streamers. This is the main avenue we explore in this work.

In this work we solve the Boltzmann equation for electron swarms undergoing ionization and attachment in mixtures of molecular N_2 and O_2. Values and general trends in the profiles of the mean energy, rate coefficients, drift velocity and diffusion tensor are reported here. A Monte Carlo simulation technique is used to calculate the spatially resolved transport properties during the development of an electron avalanche and its transition to a streamer.

2. THEORY

The governing equation describing a swarm of charged particles moving through a background of neutral molecules in electric and magnetic fields is given by Boltzmann's equation for the phase space distribution function $f(\mathbf{r},\mathbf{c},t)$:

$$\frac{\partial f}{\partial t} + \mathbf{c}\cdot\nabla f + \frac{q}{m}\left[\mathbf{E}+\mathbf{c}\times\mathbf{B}\right]\cdot\frac{\partial f}{\partial \mathbf{c}} = -J(f). \tag{1}$$

Here **r** and **c** denote, respectively, the position and velocity of the swarm particle at time *t*, *q* and *m* are the charge and mass of the swarm particle, respectively, while **E** and **B** are the electric and magnetic fields. The right hand side of (1) denotes the linear charged-particle-neutral molecule collision operator, accounting for elastic, inelastic, and non-conservative collisions.

The directional dependence of $f(\mathbf{r},\mathbf{c},t)$ in velocity space is represented by an expansion in terms of spherical harmonics:

$$f(\mathbf{r},c,t) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} f_m^{(l)}(r,c,t) Y_m^{[l]}(\hat{c}), \tag{2}$$

where $Y_m^{[l]}(\hat{c})$ are spherical harmonics and $\hat{c}$ denotes the angles of **c**. No restrictions are placed on the number of spherical harmonics nor is any particular form of the time-dependence of the expansion coefficients assumed. The speed dependence of the coefficients $f(\mathbf{r},c,t)$ is treated by an expansion about a Maxwellian at an arbitrary time-dependent basis temperature in terms of Sonine polynomials. It is assumed that the hydrodynamic stage has been reached and that spatial dependence is treated by the density gradient expansion:

$$f(\mathbf{r},\mathbf{c},t) = \sum_{s=0}^{\infty} f^{(s)}(\mathbf{c},t)\otimes(-\nabla)^s n(\mathbf{r},t). \tag{3}$$

Using the above decompositions of *f* and an implicit finite difference evaluation of time derivatives, the Boltzmann equation is transformed into a hierarchy of doubly infinite coupled inhomogeneous matrix equations for the time-dependent moments. Finite truncation of both the Sonine polynomial and spherical harmonic

expansions permit solution of this hierarchy by direct numerical inversion. Having obtained the moments, the transport coefficients and other transport properties can be calculated and their explicit expressions are given in our recent publication (Dujko et al. 2010). The reader is referred to a recent Ph.D. thesis (Dujko 2009) for a detailed discussion of a Monte Carlo simulation technique and calculation of the spatially resolved electron transport data under hydrodynamic conditions.

3. RESULTS AND DISCUSSION

We consider the reduced electric field range: 1-1000 Td (1 Td = 10^{-21} Vm^2). The abundance of O_2 in the mixture is varied systematically. The preliminary results are obtained for zero gas temperature and thermal effects on transport data will be considered in a future work. The cross sections for the electron scattering in N_2 detailed by Stojanović and Petrović 1998, and cross sections for electron scattering in O_2 developed by Itikawa et al. 1989, are implemented in this work.

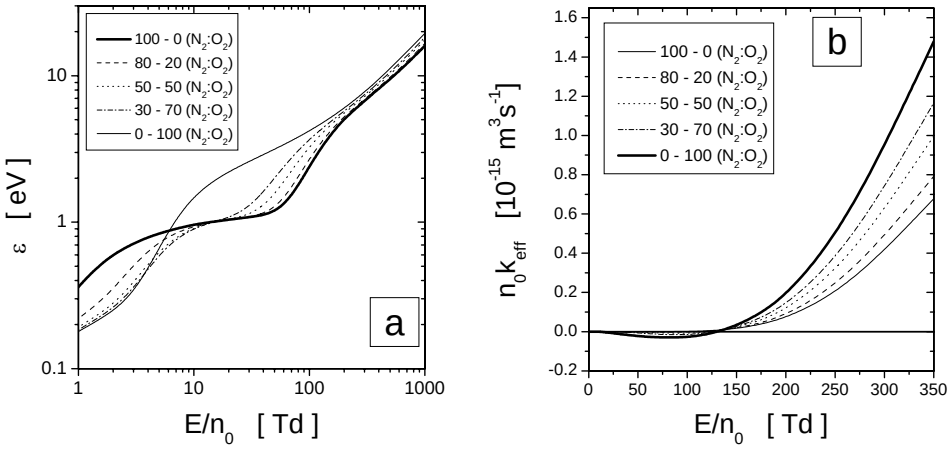

Figure 1: Variation of the mean energy (a) and effective ionization coefficient (b) with E/n_0 for various N_2-O_2 mixtures.

In Fig.1 (a) we show the mean energy as a function of E/n_0 for various N_2-O_2 mixtures. The properties of the cross sections are reflected in the profiles of the mean energy. Fig. 1 (b) displays the variation of the effective ionization coefficient with E/n_0 for various N_2-O_2 mixtures. For clarity, we show the variation of n_0k_{eff} with E/n_0 up to 350 Td. For E/n_0 less than ~135 Td and when O_2 is present, this transport property is negative, although its value is relatively small. This is a clear sign that the attachment dominates the ionization in this energy region. In the same energy region the flux values are greater than the bulk values of the drift and diffusion (not shown here). However, due to the increasing cross section for ionization and the fact that the cross section for electron attachment becomes negligible at higher energies, the effective ionization coefficient becomes positive. A

very narrow range of E/n_0 where the effective ionization coefficient passes through zero is of special interest for modeling of streamers, since it corresponds to the minimal value for the development of an electron avalanche and its transition into a streamer.

In Fig. 2 we show (a) the spatial distribution of an electron swarm and (b) average energy in the direction of electric field for various N_2-O_2 mixtures. The electron swarm is released at time $t = 0$, from a single point with a Maxwellian distribution of velocities and with a mean starting energy of 25 eV. As can be observed, the spatial profiles of the swarm relax to a Gaussian profile while the average energy has a characteristic slope. Both of these spatial distributions are significantly affected by the O_2 concentrations.

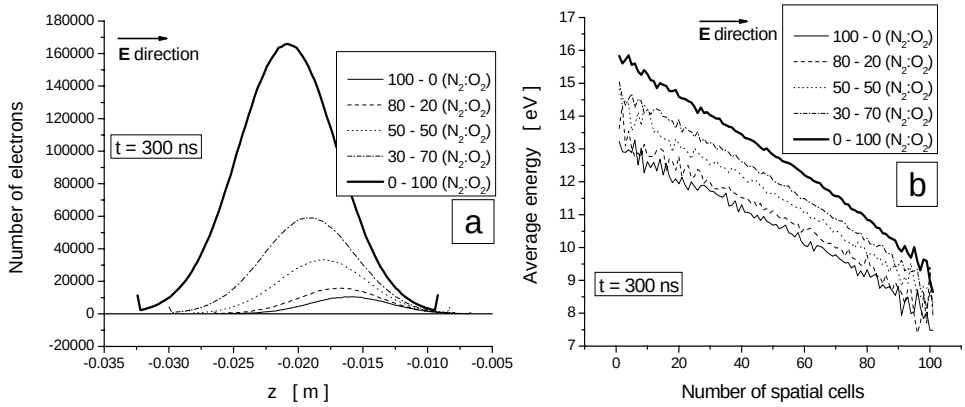

Figure 2: The spatial distribution of the electron swarm (a) and average energy (b) in the direction of the electric field for various N_2-O_2 mixtures for E/n_0 of 590 Td.

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