Научном већу Института за физику Београд

Београд, 02. фебруар 2017.

Предмет:
Покретање поступка за стицање звања истраживач сарадник

Молим Научно веће Института за физику да покрене поступак за мој избор у звање истраживач сарадник.

У прилогу достављам:

1. Мишљење руководиоца пројекта
2. Кратку стручну биографију
3. Списак објављених научних радова и њихове копије
4. Потврду о упису докторских академских студија
5. Диплому са основних и мастер студија
6. Кратак преглед научне активности

С поштовањем,
Јасмина Мирић
истраживач приправник

Мирић Јасмина

Научном већу Института за физику
Београд, 02. фебруар 2017.

Мишљење руководиоца пројекта за избор Јасмине Мирић у звање истраживач сарадник

Јасмина Мирић је запослена у Лабораторији за гасну електронику Института за физику у Београду од фебруара 2014. године. Она је ангажована на пројекту Министарства науке, просвете и технолошког развоја ИИИ41011 „Примена нискотемпературних плазми у биомедицини, заштити човекове околине и нанотехнологијама" под менторством др Саше Дујка. Кандидат је положио све испите на докторским студијама Физичког факултета на смеру Физика јонизованог гаса, плазме и технологија плазме. У периоду 2014-2016. учествовала је на међународном пројекту са једном од реномираних мултинационалних компанија.

Област научноистраживачког рада кандидата Јасмине Мирић је транспортна теорија електрона у гасовима и физика електричних гасних пражњења. На основу резултата рада Јасмине Мирић публикован је рад у међународном часопису изузетних вредности (М21а). Кандидат је био коаутор неколико уводних предавања као и радова на међународним и домаћим конференцијама. До сада постигнути резултати колегинице Мирић показују да поседује све неопходне квалитете за бављење научноистраживачким радом.

С обзиром да испуњава критеријуме предвиђене Правилником о поступку, начину вредновања и квантитативном исказивању научноистраживачких резултата истраживача Министарства просвете, науке и технолошког развоја, сагласна сам са покретањем поступка за избор Јасмине Мирић у звање истраживач сарадник.

За састав Комисије за избор Јасмине Мирић у звање истаживач сарадник предлажу се колеге:

1. др Саша Дујко, научни саветник, Институт за физику, Београд
2. проф. др Срђан Буквић, редовни професор, Физички факултет, Београд
3. академик др Зоран Љ. Петровић, научни саветник, Институт за физику, Београд

Руководилац пројекта ИИИ41011

др Невена Пуач
научни саветник,
Институт за физику, Београд

СТРУЧНА БИОГРАФИЈА

Образовање:

Јасмина Мирић је рођена 3. фебруара 1987. године у Призрену где је завршила првих шест разреда основне школе. У Београду је довршила основно образовање и завршила средњу школу.

Уписала је основне студије на Електротехничком факултету, Универзитета у Београду школске 2005/2006. године на одсеку за Физичку електронику и смеру за Биомедицински и еколошки инжињеринг. Дипломирала је са просеком 8.62 и 15. септембра 2011. године стекла звање Дипломирани инжењер електротехнике. Дипломски рад под називом "Употреба гипсаних плоча за заштиту од Рентгенског зрачења" је урађен на Електротехничком факултету под менторством проф. др Предрага Маринковића.

Мастер студије је уписала на Електротехничком факултету Универзитета у Београду школске 2011/2012. године на одсеку за Физичку електронику и смеру за Биомедицински и еколошки инжињеринг. Други степен студија је завршила са просечном оценом 10.0. Мастер рад под називом "Примене транспортних коефицијената роjева електрона у моделовању извора светлости" је урађен под менторством др Саше Дујка на Институту за физику у Београду а формални ментор на Електротехничком факултету је био проф. др Предраг Маринковић. Мастер рад је одбрањен 1. новембра 2012. године и кандидат је добио звање Мастер инжењер електротехнике и рачунарства.

Докторске студије на Физичком факултету Универзитета у Београду је уписала школске 2012/2013. године на смеру Физика јонизованог гаса, плазме и технологија плазме.

Радно искуство:

Од 5. фебруара 2014. године је запослена као истраживач приправник у Лабораторији за гасну електронику Института за физику у Београду. Ангажована је на пројекту Министарства науке, просвете и технолошког развоја ИИИ41011 „Примена нискотемпературних плазми у биомедицини, заштити човекове околине и нанотехнологијама” којим руководи др Невена Пуач.

СПИСАК ОБЈАВЉЕНИХ РАДОВА И ДРУГИХ ПУБЛИКАЦИЈА

РАД У МЕЂУНАРОДНОМ ЧАСОПИСУ ИЗУЗЕТНИХ ВРЕДНОСТИ (М21а)

1. **Jasmina Mirić**, Danko Bošnjaković, Ilija Simonović, Zoran Lj. Petrović, Saša Dujko, *Electron swarm properties under the influence of a very strong attachment in SF_6 and CF_3I obtained by Monte Carlo rescaling procedures*, Plasma Sources Sci. Technol. **25**, 065010 (2016), DOI: http://dx.doi.org/10.1088/0963-0252/25/6/065010 ISSN: 0963-0252

ПРЕДАВАЊЕ ПО ПОЗИВУ СА МЕЂУНАРОДНОГ СКУПА ШТАМПАНО У ЦЕЛИНИ (М31)

1. Saša Dujko, Danko Bošnjaković, **Jasmina Mirić**, Ilija Simonović, Zoran M. Raspopović, R. D. White, A. H. Markosyan, U. Ebert, Zoran Lj. Petrović, 9th EU-Japan Joint Symposium on Plasma Processing and EU COST MP1101 Workshop on Atmospheric Plasma Processes and Sources (JSPP2014), 19-23 January 2014, Bohinjska Bistrica, Slovenia, (Slovenian Society for Vacuum Technique) Book of Abstracts, p. INV-Dujko-1, *Recent results from studies of non-equilibrium electron transport in modeling of low-temperature plasmas and particle detectors*

ПРЕДАВАЊЕ ПО ПОЗИВУ СА МЕЂУНАРОДНОГ СКУПА ШТАМПАНО У ИЗВОДУ (М32)

1. Saša Dujko, Zoran Lj. Petrović, R. D. White, G. Boyle, Ana Banković, Ilija Simonović, D. Bošnjaković, **Jasmina Mirić**, A. H. Markosyan, Srđan Marjanović, XXIX International Conference on Photonic, Electronic and Atomic Collisions (ICPEAC2015), 22-28. July 2015, Toledo, Spain, Book of Abstracts, p. 75, *Transport processes for electrons and positrons in gases and soft-condensed matter: Basic phenomenology and applications*

2. Zoran Lj. Petrović, Saša Dujko, Dragana Marić, Danko Bošnjaković, Srđan Marjanović, **Jasmina Mirić**, Olivera Šašić, Snježana Dupljanin, Ilija Simonović, Ronald D. White, XIX International Symposium on Electron-Molecule Collisions and Swarms & XVIII International Workshop on Low-Energy Positron and Positronium Physics (POSMOL2015), 17-20. July 2015, (ISBN: 978-989-20-5845-0) Book of Abstracts, p.4, *Swarms as an exact representation of weakly ionized gases*

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   Monte Carlo simulations of electron transport in CF3I and SF6 gases

2. **Jasmina Mirić**, Ilija Simonović, Danko Bošnjaković, Zoran Lj. Petrović, Saša Dujko, Proc. 28th Summer School and International Symposium on Physics of Ionized Gases (SPIG2016), 28. August - 2. September 2016, (University of Belgrade, Faculty of Physics, Belgrade, ISBN: 978-86-84539-14-6), Book of Abstracts, p.108,
   Electron transport in mercury vapor: dimer induced NDC and analysis of transport phenomena in electric and magnetic fields

3. **Jasmina Mirić**, Olivera Šašić, Saša Dujko, Zoran Lj. Petrović,
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   Scattering Cross Sections and Transport Coefficients for Electrons in CF3I

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   Electron Transport in Noble-Gas Metal-Vapor Mixtures

5. **Jasmina Mirić**, Saša Dujko, Zoran Lj. Petrović,
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САОПШТЕЊЕ СА МЕЂУНАРОДНОГ СКУПА ШТАМПАНО У ИЗВОДУ (М34)

1. Zoran Petrović, **Jasmina Mirić**, Ilija Simonović, Danko Bošnjaković, Saša Dujko,

Bulletin of the American Physical Society, 69th Annual Gaseous Electronics Conference (GEC2016), 10-14. October 2016, (American Physical Society), Book of Abstracts, p.71, *Monte Carlo simulations of electron transport in strongly attaching gases*

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5. **Jasmina Mirić**, Danko Bošnjaković, Olivera Šašić, J. de Urquijo, Saša Dujko, Zoran Lj. Petrović,
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7. **Jasmina Mirić**, Zoran Lj. Petrović, R. D. White, Saša Dujko,

XVII International Workshop on Low-Energy Positron and Positronium Physics & XVIII International Symposium on Electron-Molecule Collisions and Swarms (POSMOL2013), 19-21. July 2013, Kanazawa, Japan, Book of Abstracts, p.46,
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Electron swarm properties under the influence of a very strong attachment in SF_6 and CF_3I obtained by Monte Carlo rescaling procedures

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Electron swarm properties under the influence of a very strong attachment in SF_6 and CF_3I obtained by Monte Carlo rescaling procedures

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Abstract

Electron attachment often imposes practical difficulties in Monte Carlo simulations, particularly under conditions of extensive losses of seed electrons. In this paper, we discuss two rescaling procedures for Monte Carlo simulations of electron transport in strongly attaching gases: (1) discrete rescaling, and (2) continuous rescaling. The two procedures are implemented in our Monte Carlo code with an aim of analyzing electron transport processes and attachment induced phenomena in sulfur-hexafluoride (SF_6) and trifluoroiodomethane (CF_3I). Though calculations have been performed over the entire range of reduced electric fields E/n_0 (where n_0 is the gas number density) where experimental data are available, the emphasis is placed on the analysis below critical (electric gas breakdown) fields and under conditions when transport properties are greatly affected by electron attachment. The present calculations of electron transport data for SF_6 and CF_3I at low E/n_0 take into account the full extent of the influence of electron attachment and spatially selective electron losses along the profile of electron swarm and attempts to produce data that may be used to model this range of conditions. The results of Monte Carlo simulations are compared to those predicted by the publicly available two term Boltzmann solver BOLSIG+. A multitude of kinetic phenomena in electron transport has been observed and discussed using physical arguments. In particular, we discuss two important phenomena: (1) the reduction of the mean energy with increasing E/n_0 for electrons in SF_6 and (2) the occurrence of negative differential conductivity (NDC) in the bulk drift velocity only for electrons in both SF_6 and CF_3I. The electron energy distribution function, spatial variations of the rate coefficient for electron attachment and average energy as well as spatial profile of the swarm are calculated and used to understand these phenomena.

Keywords: Monte Carlo, electron transport, electron attachment, SF_6, CF_3I

(Some figures may appear in colour only in the online journal)

1. Introduction

Electron transport in strongly attaching gases has long been of interest, with applications in many areas of fundamental physics and technology. Electron attaching gases support key processes for plasma etching and cleaning in semiconductor fabrication [1, 2], high-voltage gas insulation [3] and particle detectors in high energy physics [4–6]. The importance of studies of electron attachment has also been recognized in other fields, including planetary atmospheres, excimer lasers, plasma medicine and lighting applications, as well as in life science for understanding radiation damage in biological matter.

The fundamental importance of electron attachment processes has led to many experimental and theoretical swarm studies. For some gases the cross sections for attachment may be very large resulting in a rapid disappearance of free electrons that greatly complicates the measurements of transport coefficients [1, 7–9]. The pioneering studies date back to the 1970s, and the well-known swarm method of deriving cross section for electron attachment developed by Christophorou and his co-workers [10]. According to this method, trace amounts of an electron attaching gas are mixed into the buffer gases, typically nitrogen to scan the lower mean energies and argon to scan the higher mean energies. This technique results in the removal of electrons without disturbing the electron energy distribution function. In such mixtures the losses depend only on the very small amount of the added gas and we may measure the density reduced electron attachment rate coefficient. Electron attachment cross sections can be determined by deconvoluting the mixture data, since the electron energy distribution function is a known function of E/n_0 as calculated for the pure buffer gas. Examples of this procedure are cross sections for electron attachment in SF_6 and SF_6-related molecules [11–15] as well as cross sections and rate coefficients for a range of fluorocarbons [1, 12, 16–18] and other relevant gases for applications [1, 19–22]. In addition to non-equilibrium data, there is a separate category of experiments, including flowing afterglow, the Cavalleri diffusion experiment [9, 23, 24], and others that provide attachment rates for thermal equilibrium (i.e. without an applied electric field). These may be taken at different temperatures, but the range of energies covered by this technique is very narrow. These two techniques have been used to evaluate the cross sections for SF_6 and CF_3I, always under the assumption that the effect of attachment is merely on the number of particles and not on any other swarm properties.

A thorough understanding of the influence of attachment on the drift and diffusion of the electrons provides information which could be used in analysis of kinetic phenomena in complex electronegative gases and related plasmas. The attachment cooling and heating [25, 26], negative absolute electron flux mobility [27, 60] and anomalous phase shifts of drift velocity in AC electric fields [28] are some examples of these phenomena in strongly attaching gases, which may not be trivially predicted on the basis of individual collision events and external fields. Negative differential conductivity (NDC) induced by 3-body attachment for lower E/n_0 and higher pressures in molecular oxygen and its mixture with other gases is another example of phenomena induced by strong electron attachment [29]. The duality in transport coefficients, e.g. the existence of two fundamentally different families of transport coefficients, the bulk and flux, is caused by the explicit effects of electron impact ionization and electron attachment [7, 30–32]. The differences between two sets of data vary from a few percents to a few orders of magnitude and hence a special care is needed in the implementation of data in fluid models of plasma discharges [7, 31, 33–35]. On one hand, most plasma modeling is based on flux quantities while experiments aimed at yielding cross section data provide mostly but not uniquely the bulk transport data. This differentiation between flux and bulk transport properties is not merely a whimsy of theorists, but it is essential in obtaining and applying the basic swarm data. In addition, the production of negative ions has a large effect on the transport and spatial distribution of other charged particle species as well as on the structure of the sheath and occurrence of relaxation oscillations in charged particle densities [36–41].

There are three main approaches to the theoretical description of electron transport in gases: the kinetic Boltzmann equation, the stochastic particle simulation by the Monte Carlo method and semi-quantitative momentum transfer theory. Restrictions on the accuracy of momentum transfer theory for studies of electron transport in attaching gases, particularly under non-hydrodynamic conditions, have already been discussed and illustrated [31, 42, 43]. Boltzmann equation analyses for SF_6 and its mixtures with other gases (see for example [11, 44–50]) have been performed several times in the past. Two important studies devoted to the calculation of electron swarm parameters based on a Boltzmann equation have also been performed for CF_3I [51, 52]. Theories for solving the Boltzmann equation were usually restricted to low-order truncations in the Legendre expansions of the velocity dependence assuming quasi-isotropy in velocity space. The explicit effects of electron attachment were also neglected and electron transport was studied usually in terms of the flux data only. These theories had also restricted domains of validity on the applied E/n_0 in spite of their coverage of a considerably broader range. One thing that strikes the reader surveying the literature on electron transport in SF_6 is the systematic lack of reliable data for electron transport coefficients for E/n_0 less than 50 Td. Contemporary moment methods for solving Boltzmann's equation [31, 53] are also faced with a lot of systematic difficulties, particularly under conditions of the predominant removal of the lower energy electrons which results in an increase in the mean energy, i.e. attachment heating. Under these conditions the bulk of the distribution function is shifted towards a higher energy which in turn results in the high energy tail falling off much slower than a Maxwellian. This is exactly what may happen in the analysis of electron transport in strongly attaching gases such as SF_6 or CF_3I for lower E/n_0. The moment method for solving Boltzmann's equation under these circumstances usually requires the prohibitive number of basis functions for resolving the speed/energy dependency of the distribution function and/or unrealistically large computation time. As a consequence, the standard numerical schemes employed within the framework of moment methods usually fail.

The present investigation is thus mainly concerned with the Monte Carlo simulations of electron transport in strongly attaching gases. Monte Carlo simulations have also been employed for the analysis of electron transport in the mixtures of SF_6 [46, 54–57] and CF_3I [58] with other gases usually with an aim of evaluating the insulation strength and critical electric fields. However, electron attachment in strongly electronegative gases often imposes practical difficulties in Monte Carlo simulations. This is especially noticeable at lower E/n_0, where electron attachment is one of the dominant processes which may lead to the extensive vanishing of the seed electrons and

consequently to the decrease of the statistical accuracy of the output results. In extreme cases, the entire electron swarm might be consumed by attachment way before the equilibrated (steady-state regime) is achieved. An obvious solution would be to use a very large number of initial electrons, but this often leads to a dramatic increase of computation time and/or required memory/computing resources which are beyond practical limits. Given the computation restrictions of the time, the workers were forced to develop methods to combat the computational difficulties induced by the extensive vanishing of the seed electrons. Two general methods were developed: (1) addition of new electrons by uniform scaling of the electron swarm at certain time instants under hydrodynamic conditions [26, 59] or at certain positions under steady-state Townsend conditions [60], when number of electrons reaches a pre-defined threshold, and (2) implementation of an additional fictitious ionization channel/process with a constant collision frequency (providing that the corresponding ionization rate is chosen to be approximately equal to the attachment rate) [54]. On the other hand, similar rescaling may be applied for the increasing number of electrons as has been tested at the larger E/n_0 by Li *et al* [61]. Further distinction and specification between methods developed by Nolan *et al* [26] and Dyatko *et al* [60] on one hand and Raspopović *et al* [59] on the other, will be discussed in later sections. These methods have not been compared to each other in a comprehensive and rigorous manner. This raises a number of questions. How accurate, these methods are? Which is the more efficient? Which is easier for implementation? What is their relationship to each other? Which one is more flexible? In this paper, we will try to address some of these issues. In particular, the present paper serves to summarize the salient features of these methods in a way which we hope will be of benefit to all present and future developers of Monte Carlo codes. Finally, it is also important to note that in the present paper we extend the method initially developed by Yousfi *et al* [54], by introducing time-dependent collision frequency for the fictitious ionization process.

This paper is organized as follows: in section 2, we briefly review the basic elements of our Monte Carlo code, before detailing the rescaling procedures employed to combat the computational difficulties initiated by the rapid disappearance of electrons. In the same section, we illustrate the issue of electron losses by considering the evolution of the number of electrons for a range of E/n_0 in SF_6 and CF_3I. In section 3, we evaluate the performance of rescaling procedures by simulating electron transport in SF_6 and CF_3I over a wide range of E/n_0. We will also highlight the substantial difference between the bulk and flux transport coefficients in SF_6 and CF_3I. Special attention will be paid to the occurrence of negative differential conductivity (NDC) in the profile of the bulk drift velocity. For electrons in SF_6 another phenomenon arises: for certain reduced electric fields we find regions where the swarm mean energy decreases with increasing E/n_0. In the last segment of the section 3, we discuss two important issues: (1) how to use the rescaling procedures in Monte Carlo codes, and (2) rescaling procedures as a tool in the modeling of non-hydrodynamic effects in swarm experiments. In section 4, we present our conclusions and recommendations.

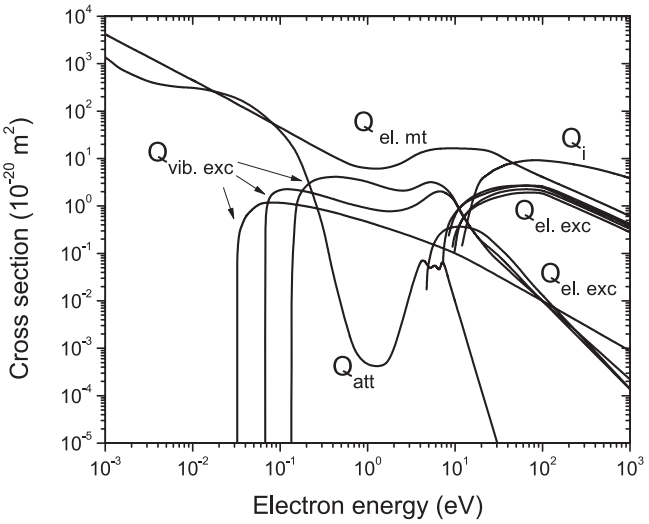

Figure 1. Electron impact cross-sections for CF_3I used in this study [62]: $Q_{el.\ mt}$ momentum transfer in elastic collisions, $Q_{vib.\ exc}$ vibrational excitation, $Q_{el.\ exc}$ electronic excitation, Q_{att} dissociative attachment and Q_i electron-impact ionization.

2. Input data and computational methods

2.1. Cross sections for electron scattering and simulation conditions

We begin this section with a brief description of cross sections for electron scattering in SF_6 and CF_3I. For the SF_6 cross sections we use the set developed by Itoh *et al* [47]. This set was initially based on published measurements of cross sections for individual collision processes. Using the standard swarm procedure, the initial set was modified to improve agreement between the calculated swarm parameters and the experimental values. The set includes one vibrational channel, one electronic excitation channel, as well as elastic, ionization and five different attachment channels.

This study considers electron transport in CF_3I using the cross section set developed in our laboratory [62]. This set of cross sections is shown in figure 1. It should be noted that this set is similar but not identical to that developed by Kimura and Nakamura [63]. We have used the measured data under pulsed Townsend conditions for pure CF_3I and its mixtures with Ar and CO_2 in a standard swarm procedure with the aim of improving the accuracy and completeness of a set of cross sections. It consists of the elastic momentum transfer cross section, three cross sections for vibrational and five cross sections for electronic excitations as well as one cross section for electron-impact ionization with a threshold of 10.4 eV and one cross section for dissociative attachment. For more details the reader is referred to our future paper [64].

For both SF_6 and CF_3I all electron scattering are assumed isotropic and hence the elastic cross section is the same as the elastic momentum transfer cross section. Simulations have been performed for E/n_0 ranging from 1 to 1000 Td. The pressure and temperature of the background gas are 1 Torr and 300 K, respectively. It should be mentioned that special care in our Monte Carlo code has been paid to proper treatment of the thermal motion of the host gas molecules and their influence

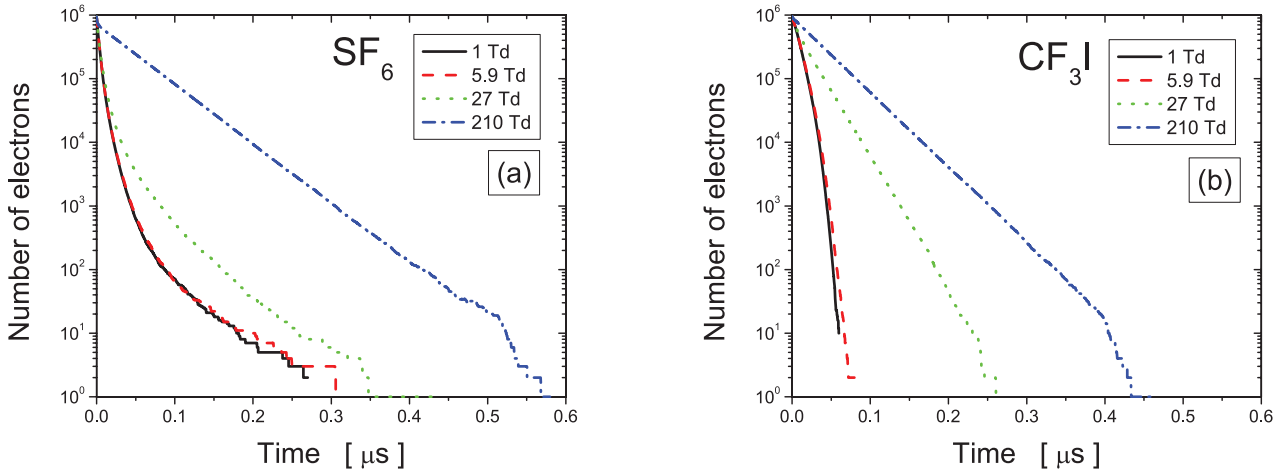

Figure 2. Electron number density decay for four different reduced electric fields as indicated on the graph. Calculations are performed for SF_6 (a) and CF_3I (b).

on electrons, which is very important at low electric fields, when the mean electron energy is comparable to the thermal energy of the host gas [65]. After ionization, the available energy is partitioned between two electrons in such a way that all fractions of the distribution are equally probable.

2.2. Monte Carlo method

The Monte Carlo simulation technique used in the present work is described at length in our previous publications [32, 53, 59, 66, 67]. In brief, we follow the spatiotemporal evolution of each electron through time steps which are fractions of the mean collision time. In association with random numbers, these finite time steps are used to solve the integral equation for the collision probability in order to determine the time of the next collision. The number of time steps is determined in such a way as to optimize the performance of the Monte Carlo code without reducing the accuracy of the final results. When the moment of the next collision is established, the additional sequences of random numbers are used, first to determine the nature of a collision, taking into account the relative probabilities of the various collision types, and second to determine the change in the direction of the electron velocity. All dynamic properties of each electron such as position, velocity, and energy are updated between and after the collisions. Sampling of electron dynamic properties is not correlated to the time of the next collision and is performed in a way that ensemble averages can be taken in both the velocity and configuration space. Explicit formulas for the bulk and flux transport properties have been given in our previous publications [59, 66]. To evaluate the accuracy of the Monte Carlo code, Boltzmann analyses were performed in parallel with the Monte Carlo calculations using the multi term method described in detail by Dujko *et al* [53]. In addition, we use the BOLSIG+, a publicly available Boltzmann solver based on a two term theory [68]. The most recent version of this code might be used to study the electron transport in terms of both the flux and bulk data which is very useful for some aspects of plasma modeling [7]. At the same time, the comparison between our results and those computed by BOLSIG+ which is presented in this paper, should be viewed as the first benchmark for the bulk BOLSIG+ data. Our Monte Carlo code and multi term codes for solving the Boltzmann equation have been subject of a detailed testing for a wide range of model and real gases [31, 53, 59, 67].

In figure 2 we illustrate the losses of electrons during the evolution of the swarm towards the steady-state. The initial number of electrons is set to 1×10^6 and calculations are performed for a range of reduced electric fields E/n_0 as indicated on the graphs. For both SF_6 and CF_3I, we observe that at small E/n_0, i.e. at low mean energies, the number of electrons decreases much faster. This is a clear sign that collision frequency for electron attachment increases with decreasing E/n_0. Electrons in CF_3I are lost continuously and consequently the number of electrons in the swarm decreases exponentially with time. The same trend may be observed for electrons in SF_6 at 210 Td. For the remaining E/n_0 the number of electrons is reduced with time even faster. Comparing SF_6 and CF_3I, it is evident that the electrons are more efficiently consumed by electron attachment in SF_6 in the early stage of the simulation. Conversely, in the last stage of simulation the electrons are more consumed by electron attachment in CF_3I than in SF_6. In any case, the electron swarms in both cases are entirely consumed by attachment way before the steady-state regime and hence the simulations are stopped. In other words, the number density drops down by six orders of magnitude over the course of several hundred nanoseconds in both gases. To facilitate the numerical simulation, it is clear that some kind of rescaling of the number density is necessary to compensate for the electrons consumed by electron attachment. This procedure should not in any way disrupt the spatial gradients in the distribution function. On the other hand, releasing electrons with some fixed arbitrary initial condition would require that they equilibrate with the electric field during which time again majority of such additional electrons would be lost.

2.3. Rescaling procedures

To counteract the effect of attachment in an optimal fashion while keeping the statistical accuracy, the following rescaling procedures were proposed and applied so far:

(1) Uniform generation of new electrons with initial properties taken from the remaining electrons thus taking advantage of the equilibration that has been achieved so far [59]. To make this procedure effective i.e. to avoid losing population in some smaller pockets of the ensemble the population should be allowed to oscillate between N_1 and N_0, where $N_1 > N_0$ but their difference is relatively small. Here N_0 is minimum allowed number of electrons while N_1 is maximum number of electrons in the simulation after rescaling.
(2) Uniform scaling of an electron swarm by a factor of 2 or 3 at certain instants of time [26] or distance [60] depending on the simulation conditions where the probability of scaling for each electron is set to unity.
(3) Introduction of an additional fictitious ionization process with a constant ionization frequency (that is close to the rate for attachment), which artificially increases the number of simulated electrons [54, 61]. Uniform rescaling of the swarm is done by randomly choosing the electrons which are to be 'duplicated'. The newborn electron has the same initial dynamic properties, coordinates, velocity, and energy as the original. Following the creation of a new electron their further histories diverge according to the independently selected random numbers.

Comparing the procedures (1) and (2), it is clear that there are no essential differences between them. The only difference lies in the fact that in the procedure (2) duplicating is performed for all the electrons in the simulation while according the procedure (1), the probability of duplication is determined by the current ratio of the number of electrons to the desired number of electrons in the simulation, which is specified in advance. On the other hand, fictitious ionization collision generates a new electron which is given the same position, velocity and energy as the primary electron that is not necessarily the electron lost in attachment. In this paper, we shall refer to the procedure (1) as *discrete rescaling*, since the procedure is applied at discrete time instants. The procedure (2) shall be termed as *swarm duplication* and finally we shall refer to the procedure (3) as the *continuous rescaling* since the rescaling is done during the entire simulation. An important requirement is that the rescaling must not perturb/change/disturb the normalized electron distribution function and its evolution. Li *et al* [61] showed that the continuous rescaling procedure meets this requirement. In case of discrete rescaling as applied to the symmetrical yet different problem of excessive ionization, it was argued that one cannot be absolutely confident that the rescaled distribution is a good representation of the original [69], except when steady state is achieved [70].

In what follows, we discuss the continuous rescaling. Following the previous works [54, 61], the Boltzmann equation for the distribution function $f(\mathbf{r}, \mathbf{c}, t)$ without rescaling and $f^\star(\mathbf{r}, \mathbf{c}, t)$ with rescaling are given by:

$$(\partial_t + \mathbf{c} \cdot \nabla_\mathbf{r} + \mathbf{a} \cdot \nabla_\mathbf{c}) f(\mathbf{r}, \mathbf{c}, t) = -J(f), \tag{1}$$

and

$$(\partial_t + \mathbf{c} \cdot \nabla_\mathbf{r} + \mathbf{a} \cdot \nabla_\mathbf{c}) f^\star(\mathbf{r}, \mathbf{c}, t) = -J(f^\star) + \nu_{\mathrm{fi}}(t) f^\star, \tag{2}$$

where $\mathbf{a}$ is the acceleration due to the external fields, $J(f)$ is the collision operator for electron-neutral collisions and ν_{fi} is time-dependent fictitious ionization rate. If the collision operator is linear (i.e. if electron–electron collisions are negligible) and if the initial distributions (at time $t = 0$) are the same, it can be easily shown that the following relationship holds

$$f^\star(\mathbf{r}, \mathbf{c}, t) = f(\mathbf{r}, \mathbf{c}, t) \exp\left(\int_0^t \nu_{\mathrm{fi}}(\tau) \mathrm{d}\tau \right). \tag{3}$$

Substituting equation (3) into equation (2) and using the linearity of the collision operator yields the following equation

$$J(f^\star) = \exp\left(\int_0^t \nu_{\mathrm{fi}}(\tau) \mathrm{d}\tau \right) J(f). \tag{4}$$

Note that in contrast to Li *et al* [61] the collision frequency for the fictitious ionization is now a time-dependent function. In terms of numerical implementation, the only difference between our continuous rescaling procedure and the one described in [54, 61] is that we do not need to provide the fictitious ionization rate which is estimated by trial and error, in advance (*a priori*). Instead, our fictitious ionization rate is initially chosen to be equal to the calculated attachment rate at the beginning of the simulation. Afterwards, it is recalculated at fixed time instants in order to match the newly developed attachment rates. As a result, the number of electrons during the simulation usually does not differ from the initial one by more than 10%. It should be noted that the fictitious ionization process must not in any way be linked to the process of real ionization. It was introduced only as a way to scale the distribution function, or in other words, as a way of duplicating the electrons.

3. Results and discussion

In this section the rescaling procedures and associated Monte Carlo code outlined in the previous section are applied to investigate transport properties and attachment induced phenomena for electrons in SF_6 and CF_3I. Electron transport in these two strongly attaching gases provides a good test of different rescaling procedures, particularly for lower E/n_0 where electron attachment is the dominant non-conservative process. In addition to comparisons between different rescaling procedures, the emphasis of this section is the observation and physical interpretation of the attachment induced phenomena in the E/n_0-profiles of mean energy, drift velocity and diffusion coefficients. In particular, we investigate the differences between the bulk and flux transport coefficients. We do not compare our results with experimentally measured data as it would distract the reader's attention to the problems associated with the quality of the sets of the cross sections for electron scattering. There are no new experimental measurements of transport coefficients for electrons in SF_6, particularly for E/n_0 less than 50 Td and thus we have deliberately chosen not to display the comparison. On the other hand, one cannot expect the multi term results to be useful here as the conditions with excessive attachment would make convergence difficult in the low E/n_0 region, where comparison would be of

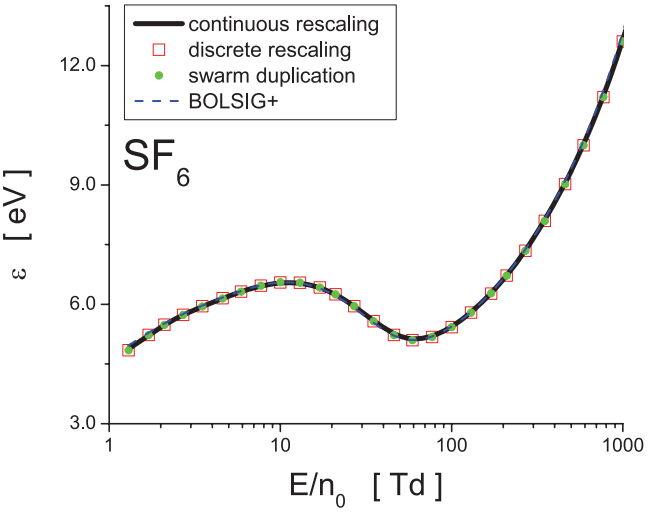

Figure 3. Variation of the mean energy with E/n_0 for electrons in SF_6. Monte Carlo results using three different techniques for electron number density compensation (rescaling) are compared with the BOLSIG+ results.

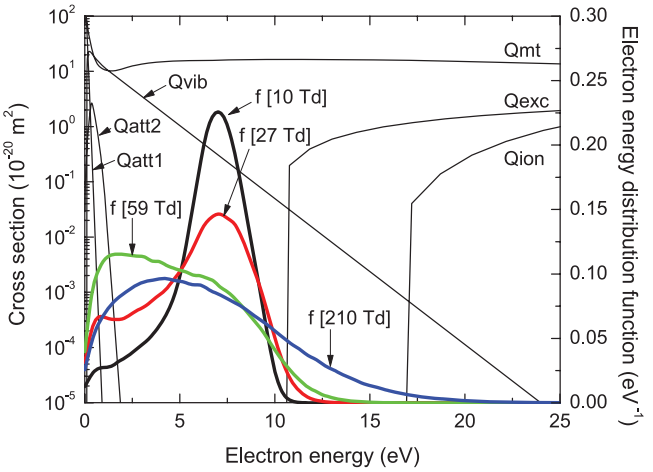

Figure 4. Electron energy distribution functions for E/n_0 of 10, 27, 59 and 210 Td. Cross sections for elastic momentum transfer (Qmt), electronic excitation (Qexc) and ionization (Qion) as well as for attachments that lead to the formation of SF_6^- (Qatt1) and SF_5^- (Qatt2) ions, are also included.

interest. Thus, for clarity the multi term results are omitted. Both experimental and theoretical work on electron swarms in SF_6 prior to 1990 is summarized in the papers of Phelps and van Brunt [11], Gallagher *et al* [71] and Morrow [72]. Recent results can be found in the book by Raju [22] and the review article of Christophorou and Olthoff [12]. The swarm analysis and further improvements of the cross sections for electron scattering in CF_3I is a subject of our future work [64].

3.1. Transport properties for electrons in SF_6 and CF_3I

3.1.1. Mean energy. In figure 3 we show the variation of the mean energy with E/n_0 for electrons in SF_6. The agreement between different rescaling procedures is excellent. This suggests that all rescaling procedures are equally valid for calculation of the mean energy (provided that rescaling is performed carefuly). In addition, the BOLSIG+ results agree very well with those calculated by a Monte Carlo simulation technique. For lower E/n_0, the mean energy initially increases with E/n_0, reaching a peak at about 10 Td, and then surprisingly it starts to decrease with E/n_0. The minimum of mean energy occurs at approximately 60 Td. For higher E/n_0 the mean energy monotonically increases with E/n_0. The reduction in the mean energy with increasing E/n_0 has been reported for electrons in Ar [73] and O_2 [74] but in the presence of very strong magnetic fields. In the present work, however, the mean energy is reduced in absence of magnetic field which certainly represents one of the most striking and anomalous effects observed in this study. Moreover, this behavior is contrary to previous experiences in swarm physics as one would expect the mean swarm energy to increase with increasing E/n_0. This is discussed in detail below.

In order to understand the anomalous behavior of the mean energy of electrons in SF_6, in figure 4 we display the electron energy distribution functions for E/n_0 at 10, 27, 59 and 210 Td. Cross sections for some of the more relevant collision processes are also included, as indicated in the graph. For clarity, the attachment cross sections for the formation of SF_4^-, F_2^- and F^- are omitted in the figure. For E/n_0 of 10 and 27 Td we observe the clear signs of 'hole burning' in the electron energy distribution function (EEDF). This phenomenon has been extensively discussed for electrons in O_2 [75, 76], O_2 mixtures [29, 77] and under conditions leading to the phenomenon of absolute negative electron mobility [27, 60] as well as for electrons in the gas mixtures of $C_2H_2F_4$, iso-C_4H_{10} and SF_6 used in resistive plate chambers in various high energy physics experiments at CERN [6]. For electrons in SF_6, the collision frequency for electron attachment decreases with energy and hence the slower electrons at the trailing edge of the swarm are preferentially attached. As a consequence, the electrons are 'bunched' in the high-energy part of the distribution function which in turn moves the bulk of the distribution function to higher energies. This is the well-known phenomenon of attachment heating which has already been discussed in the literature for model [25, 26] and real gases [6, 29]. In the limit of the lowest E/n_0 we see that due to attachment heating the mean energy attains the unusually high value of almost 5 eV. For a majority of molecular gases, however, the mean energy is significantly reduced for lower E/n_0 due to presence of rotational, vibrational and electronic excitations which have threshold energies over a wide range. As E/n_0 further increases the mean energy is also increased as electrons are accelerated through a larger potential. However, in case of SF_6, for E/n_0 increasing beyond 10 Td the mean energy is reduced. This atypical situation follows from the combined effects of attachment heating and inelastic cooling. From figure 4 we see that for E/n_0 of 27 and 59 Td the electrons from the tail of the corresponding distribution functions have enough energy to undergo the electronic excitation. Whenever an electron undergoes electronic excitations (or ionization) it loses the threshold energy of 9.8 eV (or 15.8 eV in case of ionization) and emerges from the collision with a reduced energy. This in turn diminishes the phenomenon of 'hole burning' in the distribution function by repopulating

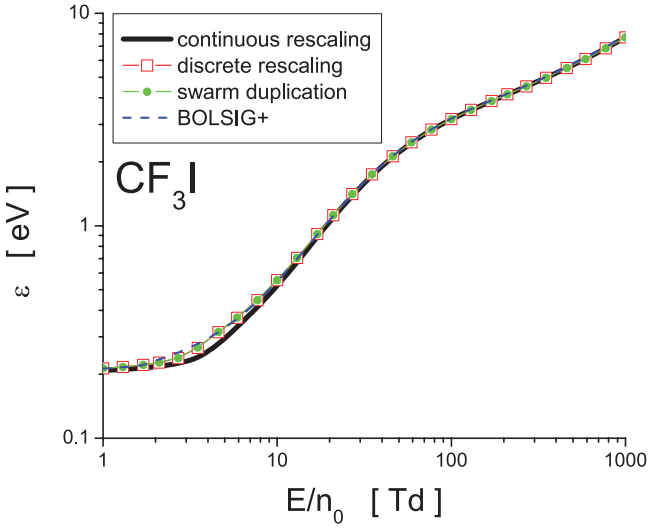

Figure 5. Variation of the mean energy with E/n_0 for electrons in CF_3I. Monte Carlo results using three different techniques for electron compensation are compared with the BOLSIG+ results.

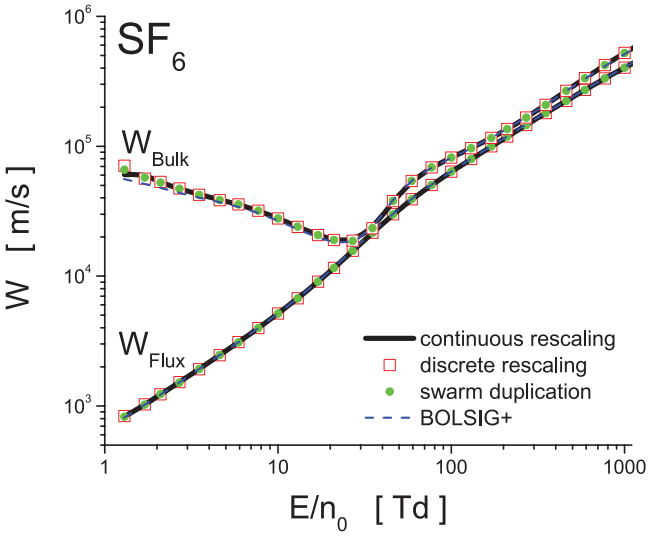

Figure 6. Variation of the drift velocity with E/n_0 for electrons in SF_6. Monte Carlo results using three different techniques for electron number density compensation are compared with the BOLSIG+ results.

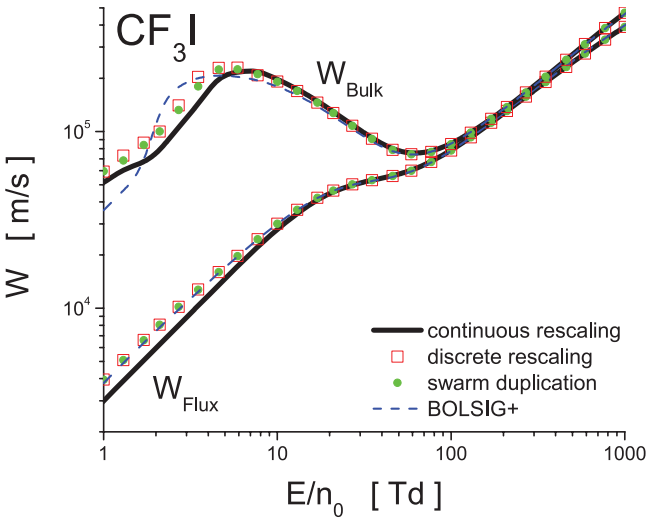

Figure 7. Variation of the drift velocity with E/n_0 for electrons in CF_3I. Monte Carlo results using three different techniques for electron number density compensation are compared with the BOLSIG+ results.

the distribution function at the lower energy. The combined effects of attachment heating and inelastic cooling and subsequent redistribution of low-energy electrons are more significant for the energy balance than the energy gain from electric field and losses in other collisions. The vibrational excitation with the threshold of 0.098 eV is of less importance having in mind the actual values of the mean energy. For E/n_0 higher than 60 Td, the dominant part in the energy balance is the energy gain from the electric field while attachment heating and induced phenomena are significantly suppressed. Thus, for E/n_0 higher than 60 Td the mean energy monotonically increases with increasing E/n_0.

The variation of the mean energy with E/n_0 for electrons in CF_3I is shown in figure 5. The agreement between different rescaling procedures is very good. Small deviations between discrete rescaling and swarm duplication from one side and continuous rescaling from the other side are present between approximately 3 and 20 Td. BOLSIG+ slightly overestimates the mean energy only in the limit of the lowest E/n_0. In contrast to mean energy of the electrons in SF_6, the mean energy of the electrons in CF_3I monotonically increases with E/n_0 without signs of anomalous behavior. If we take a careful look, then we can isolate three distinct regions of electron transport in CF_3I as E/n_0 increases. First, there is an initial region where the mean energy raises relatively slowly due to large energy loss of the electrons in low-threshold vibrational excitations. In this region the mean energy of the electrons is well above the thermal energy due to extensive attachment heating. The mean energy is raised much sharper between approximately 5 and 50 Td, indicating that electrons become able to overcome low-threshold vibrational excitations. The following region of slower rise follows from the explicit cooling of other inelastic processes, including electronic excitations and ionization, as these processes are now turned on. In conclusion, the nature of cross sections for electron scattering in CF_3I and their energy dependence as well as their mutual relations do not favor the development of the anomalous behavior of the swarm mean energy.

3.1.2. Drift velocity. In figures 6 and 7 we show variation of the bulk and flux drift velocity with E/n_0 for electrons in SF_6 and CF_3I, respectively. For electrons in SF_6 the agreement between different rescaling procedures for electron compensation is excellent for both the bulk and flux drift velocity over the entire E/n_0 range considered in this work. The BOLSIG+ bulk results slightly underestimate the corresponding bulk Monte Carlo results in the limit of the lowest E/n_0. For electrons in CF_3I, the agreement among different rescaling procedures for electron compensation is also good except for lower E/n_0 where the continuous rescaling gives somewhat lower results than other techniques.

For both SF_6 and CF_3I, we see that the bulk dominates the flux drift velocity over the entire E/n_0 range considered in this work. For lower E/n_0 this is a consequence of a very intense

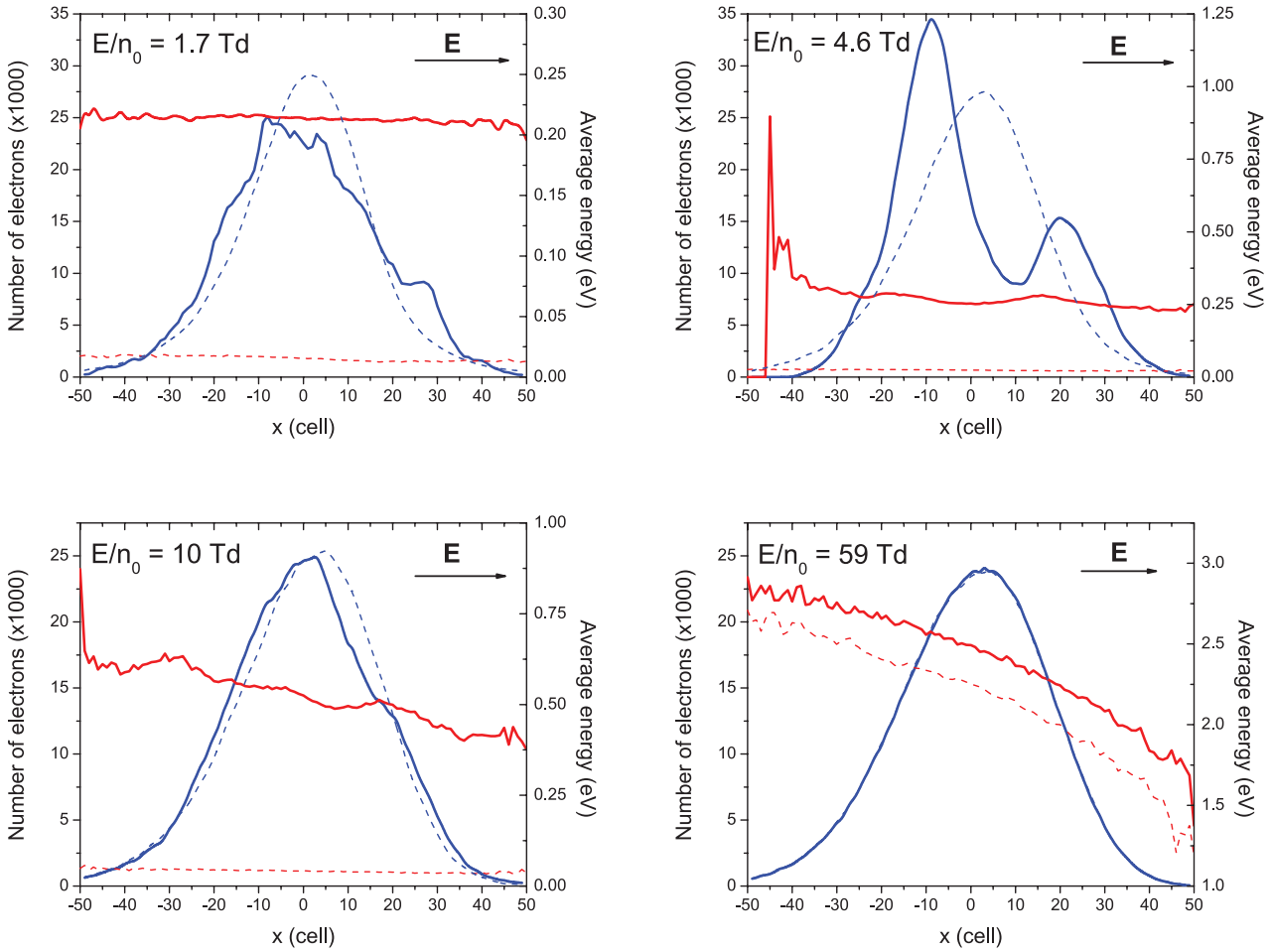

Figure 8. Spatial profile of electrons (blue curves) and spatially resolved averaged energy (red curves) at four different E/n_0 in CF_3I. Full lines denote the results when electron attachment is treated as a non-conservative process, while the dashed lines represent our results when electron attachment is treated as a conservative inelastic process with zero energy loss.

attachment heating while for higher E/n_0 this follows from the explicit effects of ionization. As mentioned above, when transport processes are greatly affected by attachment heating the slower electrons at the back of the swarm are consumed at a faster rate than those at the front of the swarm. Thus, in the case of drift, the electron attachment acts to push the centre of mass forward, increasing the bulk drift velocity above its flux component. For higher E/n_0 when ionization takes place, the ionization rate is higher for faster electrons at the front of the swarm than for slower electrons at the back of the swarm. As a result, electrons are preferentially created at the front of the swarm which results in a shift in the centre of mass. Of course, this physical picture is valid if collision frequency for ionization is an increasing function of electron energy. This is true for electrons in both SF_6 and CF_3I. The explicit effects of electron attachment are much stronger than those induced by ionization. When ionization is dominant non-conservative process, the differences between two sets of data are within 30% for both gases. When attachment dominates ionization, however, then the discrepancy between two sets of data might be almost two orders of magnitude, as for electrons in SF_6 in the limit of the lowest E/n_0.

The flux drift velocity is a monotonically increasing function of E/n_0 while the bulk component behaves in a qualitatively different fashion. A prominent feature of electron drift in SF_6 and CF_3I is the presence of a very strong NDC in the profile of the bulk drift velocity. On the other hand, a decrease in the flux drift velocity with increasing E/n_0 has not been observed. Such behavior is similar of the recently observed NDC effect for positrons in molecular gases [78, 79] where Positronium (Ps) formation plays the role of electron attachment.

In order to provide physical arguments for an explanation of NDC in the bulk drift velocity, in figure 8 we show the spatial profile and spatially resolved average energy of electrons in CF_3I. Calculations are performed for four different values of E/n_0 as indicated in the graph. The direction of the applied electric field is also shown. Two fundamentally different scenarios are discussed: (1) the electron attachment is treated as a conservative inelastic process with zero energy loss, and (2) the electron attachment is treated regularly, as a true non-conservative process. The first scenario is made with the aim of illustrating that NDC is not primarily caused by the shape of cross section for attachment but rather by the synergism of explicit and the implicit effects of the number changing nature of the process on electron transport. Sampling of spatially resolved data in our Monte Carlo simulations is performed using the continuous rescaling. The continuous rescaling produces smoother curves and in most cases it is more reliable

as compared to the discrete rescaling and swarm duplication. The results of the first scenario are presented by dashed lines while the second scenario where electron attachment is treated as a true non-conservative process, is represented by full lines.

When electron attachment is treated as a conservative inelastic process, the spatial profile of electrons has a well defined Gaussian profile with a small bias induced by the effect of electric field. The non-symmetrical feature of spatial profile is further enhanced with increasing E/n_0. While for lower E/n_0 the spatial variation of the average energy is relatively low, for higher E/n_0, e.g. for E/n_0 of 59 Td the slope of the average energy is quite high, indicating that the electron swarm energy distribution is normally spatially anisotropic. It is important to note that there are no imprinted oscillations in the spatial profile of the electrons or in the profile of the average energy which is a clear sign that the collisional energy loss is governed essentially by 'continuous' energy loss processes [32].

When electron attachment is treated as a true non-conservative process, the spatial profile and the average energy of electrons are drastically changed. For all considered reduced electric fields spatially resolved average energy is greater as compared to the case when electron attachment is treated as a conservative inelastic process. For E/n_0 of 1.7 and 4.6 Td the spatial profiles of electrons depart from a typical Gaussian shape. For 1.7 Td there is very little spatial variation in the average energy along the swarm. When $E/n_0 = 4.6$ Td, however, the spatial profile is skewed, asymmetric and shifted to the left. This shift corresponds approximately to the difference between bulk drift velocities in the two scenarios. We observe that the trailing edge of the swarm is dramatically cut off while the average energy remains essentially unaltered. At the leading edge of the swarm, however, we observe a sharp jump in the average energy which is followed by a sharp drop-off. In addition, the height of spatial profile is significantly increased in comparison to the Gaussian profile of the swarm when electron attachment is treated as a conservative inelastic process. For higher E/n_0 the signs of explicit effects of electron attachment are still present but are significantly reduced. For $E/n_0 = 10$ Td the spatial dependence of the average energy is almost linear with a small jump at the leading edge of the swarm. Comparing trailing edges of the swarms at 4.6 and 10 Td we see that for higher electric field the spatial profile of electrons is by far less cut off. This suggests that for increasing E/n_0 there are fewer and fewer electrons that are consumed by electron attachment. Finally, for $E/n_0 = 59$ Td the spatial profile of electrons is exactly the same as the profile obtained under conditions when electron attachment is treated as a conservative inelastic process.

The spatially resolved attachment rates are displayed in figure 9 and are calculated under the same conditions as for the spatial profile of the electrons and spatially averaged energy. We see that the attachment rate peaks at the trailing edge of the swarm where the average energy of the electrons is lower. Attachment loss of these lower energy electrons causes a forward shift to the swarm centre of mass, with a corresponding increase in the bulk drift velocity. For increasing E/n_0, the spatially resolved attachment rate coefficients are reduced and linearly decrease from the trailing edge towards the leading

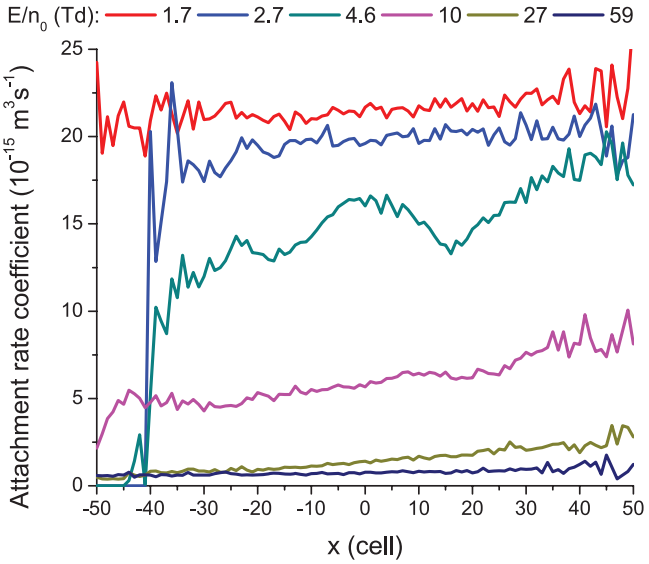

Figure 9. Spatially resolved attachment rate coefficient for a range of E/n_0 as indicated on the graph. Calculations are performed for electrons in CF_3I.

part of the swarm. At the same time the electrons at the leading edge of the swarm have enough energy to undergo ionization. This suggests much less explicit influence of electron attachment on the electron swarm behavior. As a consequence, NDC is removed from the profile of the bulk drift velocity.

In addition to the explicit effects of electron attachment there are implicit effects due to energy specific loss of electrons, which changes the swarm energy distribution as a whole, and thus indirectly changes the swarm flux. Generally speaking, it is not possible to separate the explicit from implicit effects, except by analysis with and without the electron attachment. Using these facts as motivational factors, in figure 10 we show the electron energy distribution functions for the same four values of E/n_0 considered above. The electron energy distribution functions are calculated when electron attachment is treated as a true non-conservative process (full line) and under conditions when electron attachment is assumed to be a conservative inelastic process (dashed line). As for electrons in SF_6, we observe a 'hole burning' effect in the energy distribution function which is certainly one of the most illustrative examples of the implicit effects. Likewise, we see that the high energy tail of the distribution function falls off very slowly even slower than for Maxwellian. Under these circumstances, when the actual distribution function significantly deviates from a Maxwellian, the numerical schemes for solving the Boltzmann equation in the framework of moment methods usually fail. Indeed, for E/n_0 less than approximately 20 Td we have found a sudden deterioration in the convergence of the transport coefficients which was most pronounced for the bulk properties. Furthermore, we see that the 'hole burning' effect is not present when electron attachment is treated as a conservative inelastic process. The lower energy part of the distribution function is well populated while high energy part falls off rapidly. For increasing E/n_0 and when electron attachment is treated as a true non-conservative process, the effect of hole burning is reduced markedly while

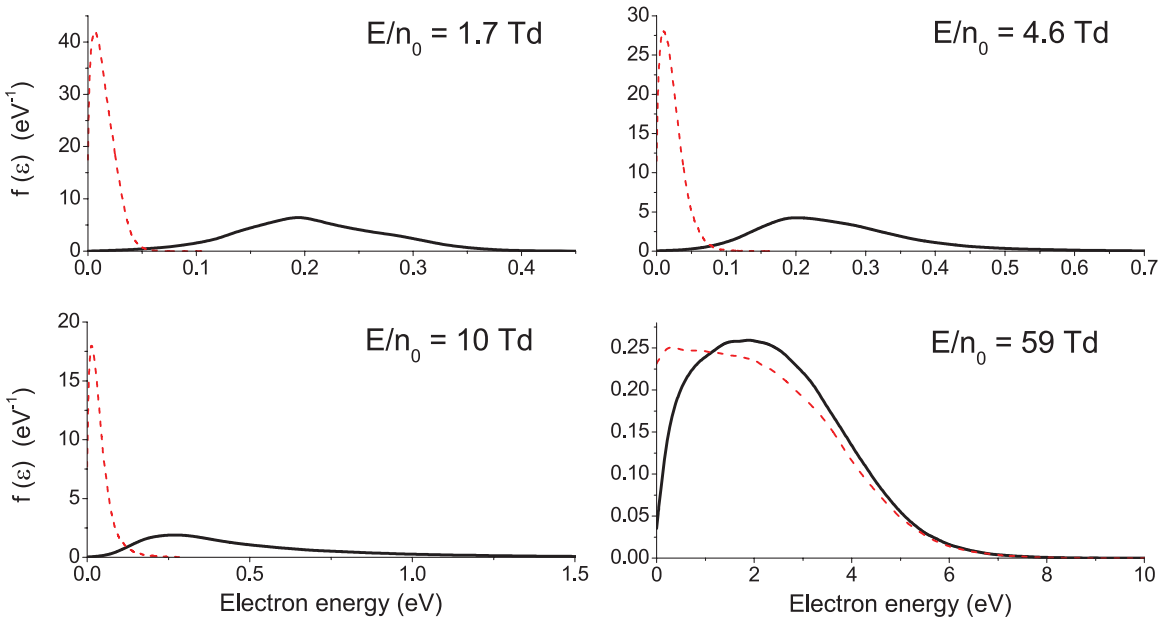

Figure 10. Energy distribution functions for four different E/n_0 for electrons in CF_3I. Black lines denote the results when electron attachment is treated as non-conservative process while dashed red lines represent our results when electron attachment is treated as a conservative inelastic process.

the high energy part of the distribution function coincides with the corresponding one when electron attachment is treated as a conservative inelastic process.

Before embarking on a discussion of our results for diffusion coefficients, one particular point deserves more mention. NDC phenomenon in the bulk drift velocity has not been experimentally verified, neither for SF_6 nor for CF_3I. On the other hand, as we have already seen, the two entirely different theoretical techniques for calculating the drift velocity predict the existence of the phenomenon. Thus, it would be very useful to extend the recent measurements of the drift velocity in both SF_6 and CF_3I to lower E/n_0 with the aim of confirming the existence of NDC. On the other hand, such measurements are most likely very difficult, even impossible due to rapid losses of electron density in experiment.

3.1.3. Diffusion coefficients. Variations of the longitudinal and transverse diffusion coefficients with E/n_0 for electrons in SF_6 are displayed in figures 11 and 12, respectively. From the E/n_0-profiles of the longitudinal and transverse flux diffusion coefficients, we observe that different rescaling procedures for Monte Carlo simulations agree very well. For the bulk components, the agreement is also very good for intermediate and higher E/n_0 and only in the limit of the lowest E/n_0 the agreement is deteriorated. Over the range of E/n_0 considered we see that there is an excellent agreement between continuous and discrete rescaling.

Comparing Monte Carlo and BOLSIG+ results, the deviations are clearly evident. They might be attributed to the inaccuracy of the two term approximation of the Boltzmann equation which is always considerably higher for diffusion than for the drift velocity. For higher E/n_0, inelastic collisions are significant and the distribution function deviates substantially from isotropy in velocity space. In these circumstances,

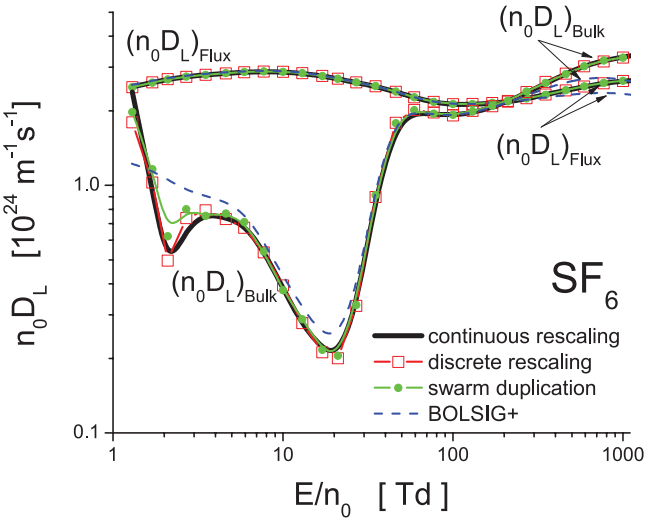

Figure 11. Variation of the longitudinal diffusion coefficient with E/n_0 for electrons in SF_6. Monte Carlo results using three different techniques for electron number density compensation are compared with the BOLSIG+ results.

the two term approximation of the Boltzmann equation fails and multi-term Boltzmann equation analysis is required. For lower E/n_0, however, the role of inelastic collisions is of less significance, but still discrepances between the BOLSIG+ and Monte Carlo results are clearly evident, particularly for the longitudinal diffusion coefficient. This suggests that further analyses of the impact of electron attachment on the distribution function in velocity space of electrons in SF_6 would be very useful.

From the profiles of the longitudinal diffusion coefficient at lower and intermediate values of E/n_0 we observe the following interesting points. In contrast to drift velocity (and transverse diffusion coefficient shown in figure 12) we see

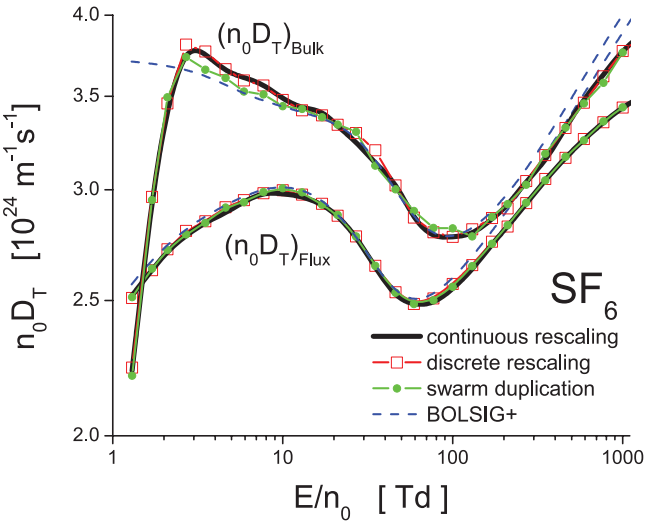

Figure 12. Variation of the transverse diffusion coefficient with E/n_0 for electrons in SF_6. Monte Carlo results using three different techniques for electron number density compensation are compared with the BOLSIG+ results.

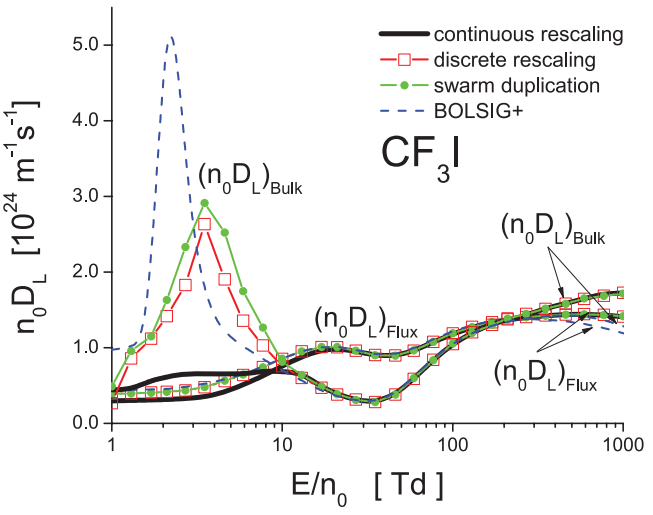

Figure 13. Variation of the longitudinal diffusion coefficient with E/n_0 for electrons in CF_3I. Monte Carlo results using three different techniques for electron number density compensation are compared with the BOLSIG+ results.

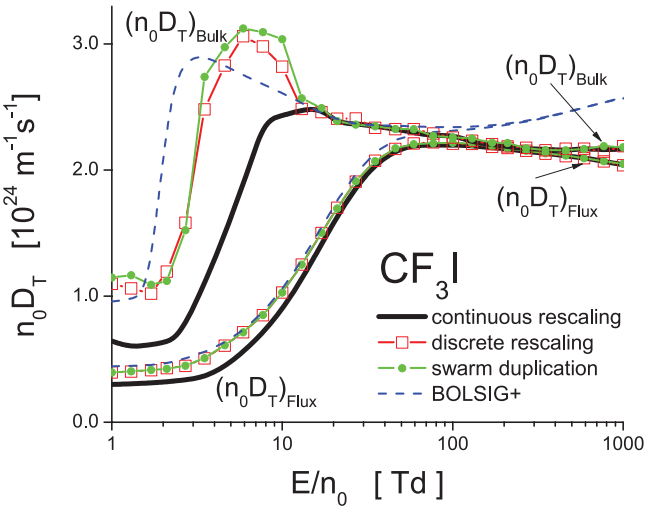

Figure 14. Variation of the transverse diffusion coefficient with E/n_0 for electrons in CF_3I. Monte Carlo results using three different techniques for electron number density compensation are compared with the BOLSIG+ results.

that the bulk diffusion coefficient is smaller than the corresponding flux component. This indicates that the decrease in electron numbers due to attachment weakens diffusion along the field direction. As already discussed, attachment loss of electrons from the trailing edge of the swarm causes a forward shift to the swarm centre of mass, with the corresponding increases in the bulk drift velocity and mean energy. The same effects result in an enhancement of the flux longitudinal diffusion. It should be noted that when attachment heating takes place, the opposite situation (bulk is higher than flux) has also been reported [25]. This is a clear sign that the energy dependence of the cross sections for electron attachment is of primary importance for the analysis of these phenomena. For higher E/n_0, however, where the contribution of ionization becomes important, we observe that the diffusion is enhanced along the field direction, e.g. the bulk dominates the flux. This is always the case if the collision frequency for ionization is an increasing function of the electron energy, independently of the gaseous medium considered.

From the profiles of the transverse diffusion coefficient the bulk values are greater than the corresponding flux values over the range of E/n_0 considered in this work. Only in the limit of the lowest E/n_0 the opposite situation holds: the flux is greater than the bulk. In contrast to the longitudinal diffusion, spreading along the transverse directions is entirely determined by the thermal motion of the electrons. The flux of the Brownian motion through a transverse plane is proportional to the speed of the electrons passing through the same plane. Therefore, the higher energy electrons contribute the most to the transversal expansion, so attachment heating enhances transverse bulk diffusion coefficient.

Figures 13 and 14 show the variations of the longitudinal and transverse diffusion coefficients with E/n_0 for electrons in CF_3I, respectively. From the E/n_0-profiles of the bulk diffusion coefficients we observe an excellent agreement between different rescaling procedures for $E/n_0 > 10$ Td. The same applies for the flux component of the longitudinal diffusion. For $E/n_0 < 10$ Td the agreement is poor for bulk components, particularly between the continuous rescaling from one side and discrete rescaling and/or swarm duplication from the other side. The agreement is better for the flux components.

Comparing Monte Carlo and BOLSIG + results, we see that the maximum error in the two term approximation, for both diffusion coefficients occurs at lower and higher E/n_0. In contrast to SF_6, CF_3I has rapidly increasing cross sections for vibrational excitations in the same energy region where the cross section of momentum transfer in elastic collisions decreases with the electron energy. Under these conditions, the energy transfer is increased and collisions no longer have the effect of randomizing the direction of electron motion. As a consequence, the distribution function deviates significantly from isotropy in velocity space and two term approximation of the Boltzmann equation fails.

When considering the differences between the bulk and flux values of diffusion coefficients the situation is much more complex comparing to SF_6. From the E/n_0-profiles of the longitudinal diffusion coefficient one can immediately see that for lower and higher E/n_0, the bulk is greater than the corresponding flux values while at intermediate E/n_0 the opposite situation holds: the flux is greater than the bulk. The behavior of the transverse diffusion coefficient is less complex, as over the entire of E/n_0 the bulk is greater that the corresponding flux values.

As we have demonstrated, in contrast to drift velocity the behavior and differences between the bulk and flux diffusion coefficients is somewhat harder to interpret. This follows from the complexity of factors which contribute to or influence the diffusion coefficients. The two most important factors are the following: (a) the thermal anisotropy effect resulting from different random electron motion in different directions; and (b) the anisotropy induced by the electric field resulting from the spatial variation of the average energy and local average velocities throughout the swarm which act so as to either inhibit or enhance diffusion. Additional factors include the effects of collisions, energy-dependent total collision frequency, and presence of non-conservative collisions. Couplings of these individual factors are always present and hence sometimes it is hard to elucidate even the basic trends in the behavior of diffusion coefficients. In particular, to understand the effects of electron attachment on diffusion coefficients and associated differences between bulk and flux components, the variation in the diffusive energy tensor associated with the second-order spatial variation in the average energy with E/n_0 should be studied. This remains the program of our future work.

3.1.4. Rate coefficients. In figure 15 we show the variation of steady-state Townsend ionization and attachment coefficients with E/n_0 for electrons in SF_6. The agreement between different rescaling procedures and BOLSIG+ code is very good. It is important to note that the agreement is very good, even in the limit of the lowest E/n_0 considered in this work where the electron energy distribution function is greatly affected by electron attachment. The curves show expected increase in α/n_0 and expected decrease in η/n_0, with increasing E/n_0. The value obtained for critical electric field is 361 Td which is in excellent agreement with experimental measurements of Aschwanden [80].

In figure 16 we show variation of the steady-state Townsend ionization and attachment coefficients with E/n_0 for electrons in CF_3I. The agreement between different rescaling procedure and BOLSIG+ code is excellent for ionization coefficient. From the E/n_0-profile of attachment coefficient, we see that the continuous rescaling slightly overestimates the remaining scenarios of computation. The critical electric field for CF_3I is higher than for SF_6. This fact has been recently used as a motivational factor for a new wave of studies related to the insulation characteristics of pure CF_3I and its mixture with other gases, in the light of the present search for suitable alternatives to SF_6. The value obtained for critical electric field in our calculations is 440 Td which is in close agreement with experimental measurements under steady-state [63, 81]

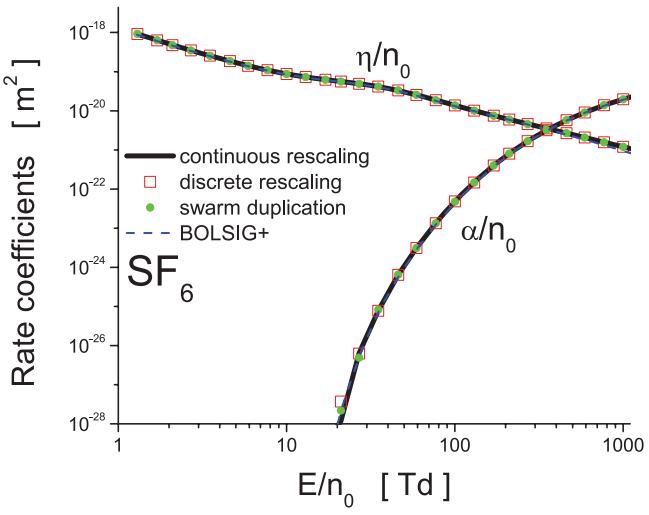

Figure 15. Variation of the rate coefficients with E/n_0 for electrons in SF_6. Monte Carlo results using three different techniques for electron number density compensation are compared with the BOLSIG+ results.

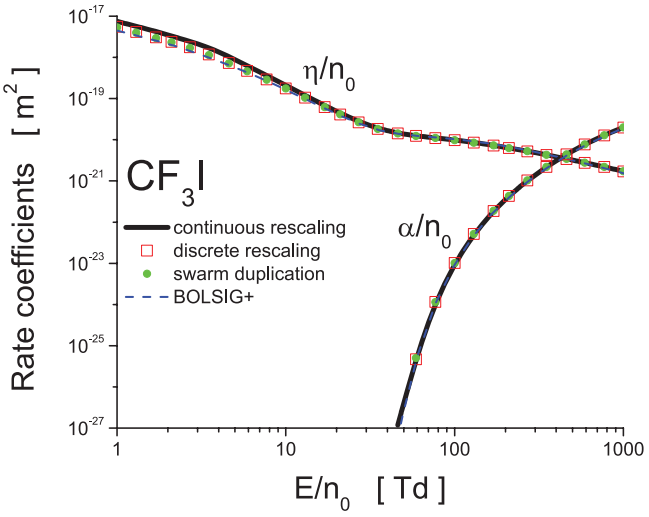

Figure 16. Variation of the rate coefficients with E/n_0 for electrons in CF_3I. Monte Carlo results using three different techniques for electron number density compensation are compared with the BOLSIG+ results.

and pulsed-Townsend [82] conditions, as well as with recent calculations performed by Kawaguchi *et al* [58] and Deng and Xiao [52].

3.2. Recommendations for implementation

In this section, we discuss the main features of the rescaling procedures and we give recommendations on how to use them in future Monte Carlo codes. Based on our experience achieved by simulating the electron transport in SF_6, CF_3I and other attaching gases, we have observed that if correctly implemented the procedures generally agree very well. The agreement between different rescaling procedures is always better for the flux than for the bulk properties. We found a poor agreement for the bulk diffusion coefficients, particularly for the lower E/n_0 while for mean energy, drift velocity and

rate coefficients the agreement is reasonably good. For lower E/n_0 when the distribution function is extremely affected by electron attachment, the agreement between swarm duplication and discrete rescaling is also good. This is not surprising as these two techniques are essentially the same.

In terms of implementation, the Monte Carlo codes can be relatively easily upgraded with the procedures for swarm duplication and/or discrete rescaling. Special attention during the implementation of these procedures should be given to the choice of the length of time steps after which the cloning of the electrons is done. If the length of this time step appears to be too long as compared to the time constant which corresponds to the attachment collision frequency, then the distribution function could be disturbed due to a low statistical accuracy. In other words, depleting certain pockets of the EEDF means that those cannot be recovered at all. On the other hand, if the length of the time steps is too small, the speed of simulation could be significantly reduced. The implementation of the continuous rescaling procedure is somewhat more complicated.

Which procedure is, the most flexible? It is difficult to answer this question because the answer depends on the criteria of flexibility. If the criterion for flexibility is associated with the need for *a priori* estimates which are necessary for setting the simulation, then the technique of continuous rescaling is certainly the most flexible. Once implemented, and thoroughly tested this procedure allows the analysis of electron transport in strongly attaching gases regardless of the energy dependence of the cross section for electron attachment. On the other hand, for the analysis of electron transport in weakly attaching gases, the discrete rescaling is very convenient because it is easier for implementation into the codes and less demanding in terms of the CPU time.

In terms of reliability and accuracy, the comparison of the results obtained for various transport properties using the rescaling procedures for Monte Carlo simulations and the Boltzmann equation codes shows that the rescaling procedures described herein are highly reliable. It should be noted that only the multi term codes for solving the Boltzmann equation may offer the final answer. Restrictions of the TTA for solving the Boltzmann equation were demonstrated many times in the past [7, 31], especially when it comes to the calculations of diffusion coefficients. Testing and benchmarking against other Boltzmann solvers are currently ongoing.

3.3. Experiments in strongly attaching gases: difficulties induced by non-hydrodynamic effects

It must be noted at this point that most processes scale with pressure, so the independence on pressure would be maintained and so would be the equilibration of EEDFs affected by excessive attachment. Most of the processes fall into that category. These processes are best visualized in an infinite uniform environment. Standard swarm experiments are built in such a way that boundaries are not felt over appreciable volume and thus, they mimic hydrodynamic conditions very well. However, going to high E/n_0 requires operating at lower pressures and there the boundaries may be felt over a larger portion of the volume. In general, whenever boundaries of any kind are introduced selective losses resulting in very different mean free paths of different groups of particles may lead to selective losses. The resulting holes in the distribution may be filled in by collisions, so when considerable selective losses are introduced results may become the pressure dependent (even when the cross section is not dependent on the pressure). The same is true for temporal limitations. For example, if the frequency of collisions is small, so that the mean free time is comparable to the time required to accelerate to energies where cross sections decrease with the electron energy, the runaway effects may be developed. Similar effects may be created due to temporal variations of the field that do not allow full equilibration. The pressure dependence of the results will develop under such conditions (and so would the dependence on the size of the vessel). The development of a non-hydrodynamic theory for solving the Boiltzmann equation is difficult and the best solution is a Monte Carlo simulation technique. For that reason, rescaling procedures are essential in modeling of the non-hydrodynamic (non-local) development of charged particle ensembles.

Experiments in gases with a very large attachment (typically at low energies) may be difficult to carry out due to a large loss of electrons. The fact that experiments in diluted gas mixtures of such gases may be feasible, means that cross sections may be obtained. Yet, one should be aware of two main problems. Even in such mixtures and depending on the size of the experiment, attachment may be high enough to induce depletion of the distribution function thus making results pressure dependent or abundance dependent. If one wants to extend the calculations to pure attaching gas for smaller vessels and pressures, one needs to be aware that only techniques that take full non-hydrodynamic description of the swarm development, are required. Similar effects have been observed in gases always associated with strong attachment such as oxygen [76] and water vapor [83]. In any case, the critical effects that include NDC for bulk drift velocity as a result of excessive loss of electrons in attachment can be observed in gases like SF_6 and CF_3I based on hydrodynamic expansion and even based on the two term theory provided that theory takes into account the explicit and implicit non-conservative effects of the attachment.

4. Conclusion

In this paper, we have presented the development, implementation and benchmarking of the rescaling procedures for Monte Carlo simulations of electron transport in strongly attaching gases. The capabilities of the rescaling procedures have been described by systematic investigation of the influence of electron attachment on transport coefficients of electrons in SF_6 and CF_3I. Among many important points, the key results arising from this paper are:

(1) We have presented two distinctively different methods for compensation of electrons in Monte Carlo simulations of electron transport in strongly attaching gases, e.g. the discrete and the continuous procedures. In order to avoid the

somewhat arbitrary choice of the fictitious ionization rate, we have extended the continuous rescaling procedure, initially developed by Li *et al* [61], by introducing a time-dependent collision frequency for the fictitious ionization process.

(2) One of the initial motivating factors for this work was to provide accurate data for transport properties of electrons in SF_6 and CF_3I which are required as input in fluid models of plasma discharges. In this work, for the first time, we have calculated the mean energy, drift velocity and diffusion coefficients as well as rate coefficients for lower E/n_0 for electrons in SF_6 and CF_3I.

(3) We have demonstrated the differences which can exist between the bulk and flux transport coefficients and the origin of these differences. Our study has shown that the flux and bulk transport properties can vary substantially from one another, particularly in the presence of intensive attachment heating. Thus, one of the key messages of this work is that theories which approximate the bulk transport coefficients by the flux are problematic and generally wrong.

(4) We have demonstrated and interpreted physically the phenomenon of the anomalous behavior of the mean energy of electrons in SF_6, in which the mean energy is reduced for increasing E/n_0. The phenomenon was associated with the interplay between attachment heating an inelastic cooling. The same phenomenon has not been observed for electrons in CF_3I indicating that the role of the cross sections is vital.

(5) We have explained and identified a region of NDC in the bulk drift velocity, originating from the explicit influence of electron attachment. The phenomenon has been explained using the concept of spatially-resolved transport properties along the swarm.

(6) The publicly available two term Boltzmann solver, BOLSIG+, has been shown to be accurate for calculations of mean energy, drift velocity and rate coefficients for electrons in SF_6 and CF_3I. On the other hand, significant differences between our Monte Carlo and BOLSIG+ results for diffusion coefficients have been observed, particularly for electrons in CF_3I in the limit of the lowest E/n_0 considered in this work.

Various rescaling procedures for Monte Carlo simulations described in this work have recently been applied to modeling of electron transport in strongly attaching gases under the influence of time-dependent electric and magnetic fields. It will be challenging to investigate the synergism of magnetic fields and electron attachment in radio-frequency plasmas. Likewise, the remaining step to be taken, is to apply the rescaling procedures presented in this work to investigate the influence of positronium formation on the positron transport properties. This remains the focus of our future investigation. Finally, we hope that this paper will stimulate further discussion on methods of correct representation of the effects induced by electron attachment on transport properties of electrons in strongly attaching gases.

Acknowledgments

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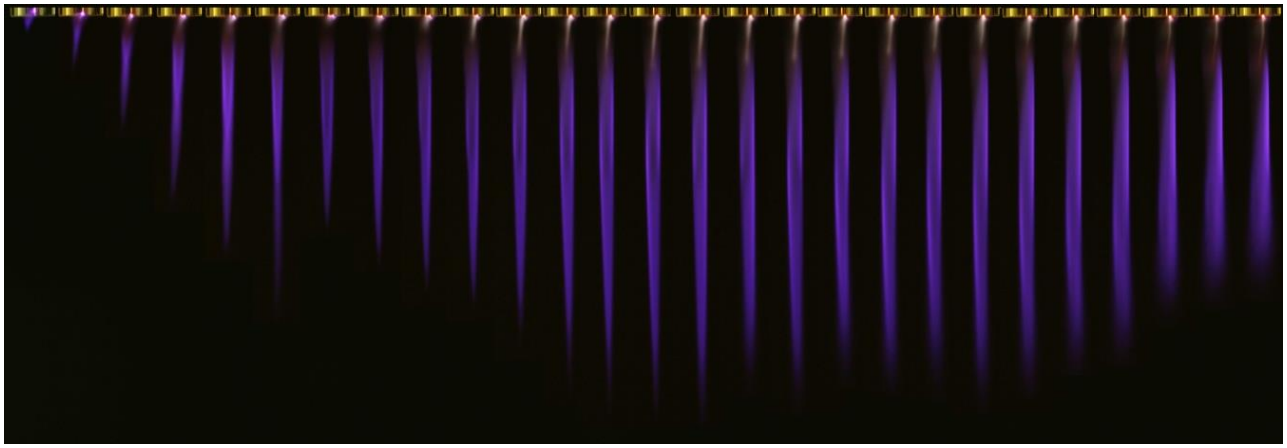

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January 19th — January 23th 2014, Bohinjska Bistrica, Slovenia

Programme and abstracts

Click on the title of a talk to see the abstract.

The 9th EU-Japan Joint Symposium on Plasma Processesing (19.-23. January 2014, Slovenia)

Sun. 19. Jan			
15.00 - 17.00	**Registration**		
17.00 - 17.30	**INV**	**S. Milošević** (CRO); Tailoring plasma sources and their diagnostics in various applications	slobodan@ifs.hr
17.30 - 18.00	**INV**	**M. Gorjanc** (SLO); Advantages and limitations of using plasma technology for modification of textiles	marija.gorjanc@ntf.uni-lj.si
18.00 - 18.30	**INV**	**K. Kutasi** (HUN); Layer-by-layer assembly of thin organic films on PTFE activated by air diffuse coplanar surface barrier discharge	kutasi.kinga@wigner.mta.hu
19.00 - 20.00	**Dinner**		
20.00 - 23.00	**Welcome reception**		

Mon. 20. Jan			
8.50 - 9.00	**Opening**	**S. Hamaguchi (JPN), U. Cvelbar (SLO)**	
9.00 - 9.45	**Plenary**	**T. Makabe** (JPN); Local distribution of gas temperature in an atmospheric- pressure microcell plasma in Ar	makabe@mkbe.elec.keio.ac.jp
9.45 - 10.30	**Plenary**	**M. M. Turner** (IRE); Uncertainty and error in complex plasma chemistry models	miles.turner@dcu.ie
10.30 - 11.00	**Break**		
11.00 -11.30	**INV**	**S. Hamaguchi** (JPN); Nano-scale damage formation during plasma etching analysed by multi-beam experiments and molecular dynamics (MD) simulations	hamaguch@ppl.eng.osaka-u.ac.jp
11.30 - 12.00	**INV**	**S. Dujko** (SRB); Recent results from studies of non-equilibrium electron transport in modelling of low-temperature plasmas and particle detectors	sasha@ipb.ac.rs
12.00 - 12.30	**INV**	**T. Murakami** (JPN); Reactive species in atmospheric pressure plasmas operated in ambient humid air	murakami@es.titech.ac.jp
12.30 - 13.00	**INV**	**M. Sekine** (JPN); Plasma nano-interface with organic materials for surface roughness formation	sekine@nagoya-u.jp
13.00 - 14.15	**Lunch**		
14.15 - 15.00	**Plenary**	**M. Shiratani** (JPN); Nanoparticle composite plasma CVD films - Fundamental and applications	siratani@ed.kyushi-u.ac.jp
15.00 - 15.30	**INV**	**R. Hatakeyama** (JPN); Plasma-processed control of graphene nanostructures and transport properties	hatake@ecei.tohoku.ac.jp
15.30 - 16.00	**INV**	**J. Kim** (JPN); Microwave plasma CVD technologies for the synthesis of nanocrystalline diamond and graphene films	jaeho.kim@aist.go.jp
16.00 – 16.30	**Break**		

Recent results from studies of non-equilibrium electron transport in modeling of low-temperature plasmas and particle detectors

S. Dujko[1], D. Bošnjaković[1], J. Mirić[1], I. Simonović[1], Z.M. Raspopović[1], R.D. White[2], A.H. Markosyan[3], U. Ebert[3] and Z.Lj. Petrović[1]

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A quantitative understanding of charged particle transport processes in gases under highly non-equilibrium conditions is of interest from both fundamental and applied viewpoints, including modeling of non-equilibrium plasmas and particle detectors used in high energy physics. In this work we will highlight how the fundamental kinetic theory for solving the Boltzmann equation [1] and fluid equations [2,3] as well as Monte Carlo simulations [3], developed over many years for charged particle swarms are presently being adapted to study the various types of non-equilibrium plasma discharges and particle detectors.

Non-equilibrium plasma discharges sustained and controlled by electric and magnetic fields are widely used in materials processing [4]. Within these discharges the electric and magnetic fields can vary in space, time and orientation depending on the type of discharge. Moreover, the typical distances for electron energy and momentum relaxation are comparable to the plasma source dimensions. Consequently, the transport properties at a given point are usually no longer a function of instantaneous fields. This is the case for a variety of magnetized plasma discharges where, before the electrons become fully relaxed, it is likely that the electrons will be

reflected by the sheath or collide with the wall [5]. In this work we will illustrate various kinetic phenomena induced by the spatial and temporal non-locality of electron transport in gases. Two particular examples of most recent interest for the authors are the magnetron and ICP discharges. The magnetron discharge is used in the sputtering deposition of in films [6] where magnetic field confines energetic electrons near the cathode. These confined electrons ionize neutral gas and form high density plasma near the cathode surface while heavy ions and neutrals impinge on the solid surface ejecting material from that surface which is then deposited on the substrate. Within these discharges the angle between the electric and magnetic fields varies and thus for a detailed understanding and accurate modeling of this type of discharge, a knowledge of electron transport in gases under the influence of electric and magnetic fields at arbitrary angles is essential. In this work we will investigate the electron transport in N_2-O_2 mixtures when electric and magnetic fields are crossed at arbitrary angles for a range of pressures having in mind applications for low-pressure magnetized discharges and discharges at atmospheric pressure. Special attention is placed upon the explicit effects of three-body attachment in oxygen on both the drift and diffusion in low energy range [7]. The duality of transport coefficients arising from the explicit effects of non-conservative collisions will be discussed not only for vectorial and low-order tensorial transport coefficients but also for the high-order tensorial transport properties. The errors associated with the two-term approximation and inadequacies of Legendre polynomial expansions for solving the Boltzmann equation will be illustrated and highlighted.

In addition to magnetron discharges, we focus on the time-dependent behavior of electron transport properties in ICP discharges where electric and magnetic fields are radiofrequency. We systematically investigate the explicit effects associated with the electric and magnetic fields including field to density ratios, field frequency to density ratio, field phases and field orientations. A multitude of kinetic phenomena were observed that are generally inexplicable through the use of steady-state dc transport theory. Phenomena of significant note include the existence of transient

negative diffusivity, time-resolved negative differential conductivity and anomalous anisotropic diffusion. Most notably, we propose a new mechanism for collisional heating in inductively coupled plasmas which results from the synergism of temporal non-locality and cyclotron resonance effect. This mechanism is illustrated for discharges in pure CF_4 and pure O_2.

As an example of fluid modeling of plasmas, we will discuss the recently developed high order fluid model for streamer discharges [2,3]. Starting from the cross sections for electron scattering, it will be shown how the corresponding transport data required as input in fluid model should be calculated under conditions when the local field approximation is not applicable. The temporal and spatial evolution of electron number density and electric field in the classical first order and in the high order model are compared and the differences will be explained by physical arguments. We will illustrate the non-local effects in the profiles of the mean energy behind the streamer front and emphasize the significance of the energy flux balance equation in modeling. We consider the negative planar ionization fronts in molecular nitrogen and noble gases. Our results for various streamers properties are compared with those obtained by a PIC/Monte Carlo approach. The comparison confirms the theoretical basis and numerical integrity of our high order fluid model for streamers discharges.

In the last segment of this talk we will discuss the detector physics processes of resistive plate chambers and time-projection chambers that are often used in many high energy physics experiments [8]. For resistive plate chambers the critical elements of modeling include the primary ionization, avalanche statists and signal development. The Monte Carlo simulation procedures that implement the described processes will be presented. Time resolution and detector efficiency are calculated and compared with experimental measurements and other theoretical calculations. Among many critical elements of modeling for time-projection chambers, we have investigated the sensitivity of electron transport properties to the pressure and temperature variations in the mixtures of Ne and CO_2. In particular, we have investigated how to reduce

the transverse diffusion of electrons by calculating the electron trajectories under the influence of parallel electric and magnetic fields and for typical conditions found in these detectors.

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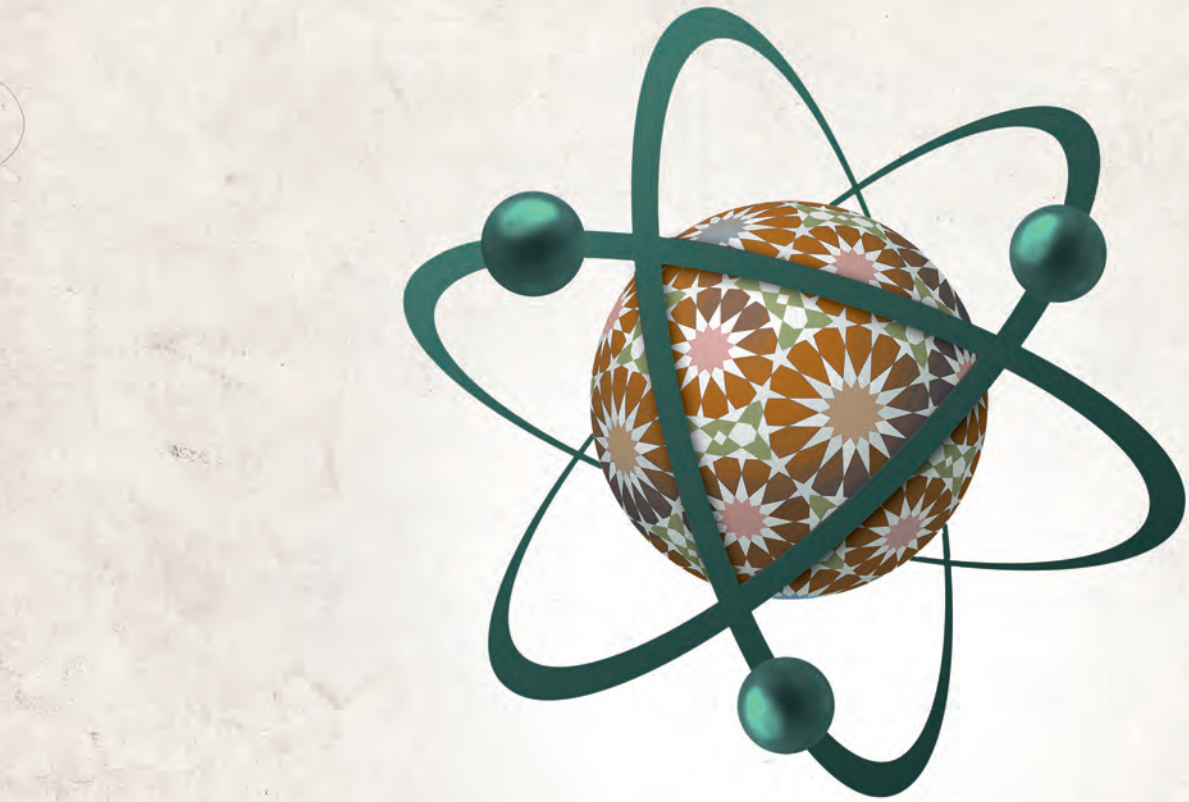

PR

Transport processes for electrons and positrons in gases and soft-condensed matter: Basic phenomenology and applications

S. Dujko* [1], **Z.Lj. Petrović***, **R.D. White**†, **G. Boyle**†, **A. Banković***, **I. Simonović***, **D. Bošnjaković***, **J. Mirić***, **A.H. Markosyan**♥ **and S. Marjanović***

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Synopsis An understanding of electron and positron transport in gases and soft-condensed matter under non-equilibrium conditions finds applications in many areas, from low-temperature plasmas, to positron emission tomography, radiation damage and particle detectors in high-energy physics. In this work we will highlight how the fundamental kinetic theory for solving the Boltzmann equation and fluid equation models are presently being adapted to study the various types of non-equilibrium plasma discharges and positron-based technologies.

The transport theory of electrons and positrons in gases and soft-condensed matter is of interest both as a problem in basic physics and for its potential for application to modern technology. For electrons, these applications range from low-temperature plasmas to particle detectors in high energy physics and to understanding radiation damage in biological matter. For positron based systems, the emission of back-to-back gamma rays resulting from annihilation of a positron and an electron is a fundamental process used as a tool in many areas, ranging from fundamental atomic and molecular physics, particle and astrophysics, to diagnostics in biological and material sciences.

In this work we explore analytical framework and numerical techniques for a multi term solution of Boltzmann's equation [1], for both electrons and positrons in gases and soft-condensed matter, and associated fluid equation models [2,3]. Together with the basic elements of our Monte Carlo method, the particular attention will be placed upon the rescaling procedures for compensation of electrons for losses under conditions when transport is greatly affected by electron attachment in strong electronegative gases.

For electrons, we will highlight recent advancements in the determination of the high-order transport coefficients in both atomic and molecular gases. Then we will discuss the elementary physical processes of electrons in the mixtures of gases used to model planetary atmospheric discharges. In particular, we will present the results of our theoretical calculations for expected heights of occurrence of sprites above lightning discharges in atmospheres of planets in our Solar system.

As an example of fluid equation models, we will discuss the recently developed high order fluid model for streamer discharges [3]. The balance equations for electron density, average electron velocity, average electron energy and average electron energy flux have been obtained as velocity moments of Boltzmann's equation and are coupled to the Poisson equation for the space charge electric field. Starting from the cross sections for electron scattering, it will be shown how the corresponding transport data required as input in fluid model should be calculated under conditions when the local field approximation is not applicable. We will illustrate the non-local effects in the profiles of the mean energy behind the streamer front and emphasize the significance of the energy flux balance equation in modeling. Numerical examples include the streamers in N_2 and noble gases.

In the last segment of this talk we will discuss the interaction of primary positrons, and their secondary electrons, with water vapor and its mixture with methane using complete sets of cross sections having bio-medical applications in mind [4]. We will also highlight recent advancements in the testing/validation of complete cross section sets for electrons in biologically relevant molecules, including water vapor and tetrahydrofuran [5].

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MONDAY

EMS

XIX International Symposium on Electron-Molecule Collisions and Swarms

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ABSTRACT INDEX

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ABSTRACT INDEX

PL-04

Swarms as an exact representation of weakly ionized gases

Zoran Lj. Petrović[1], Saša Dujko[1], Dragana Marić[1], Danko Bošnjaković[1], Srđan Marjanović[1], Jasmina Mirić[1], Olivera Šašić[1], Snježana Dupljanin[1], Ilija Simonović[1], Ronald D. White[2]

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Often swarms are regarded as idealized ensembles of charged particles that may be realized in specialized experiments to provide accurate transport coefficients, which after some analysis, yield "complete" sets of cross sections and accurate representations of non-equilibrium electron energy distribution function (EEDF) for a given *E/N*. Generally it is believed nowadays that swarms are just a tool for modeling non-equilibrium (low temperature) plasmas, as some kind of an interface through which atomic physics enters plasmas. In this review we shall show some new results that extend that picture into several directions:

- New results for the cross sections in systems where information from beam experiments and binary collision theories are insufficient such as $C_2H_2F_4$ that is commonly used as a cooling gas in modern refrigerators and air conditioners, but also it is used in particle detectors and has a potential for plasma processing applications.
- Ionized gases where swarms are exact representation of the system. Those include weakly ionized gases such as atmosphere, gas breakdown, afterglow (after the breakup of the ambipolar field), steady state Townsend regime of discharges, conduction of electricity through gases, interaction of secondary electrons produced by high energy particles with the gas or liquid background and many more. A special example will be modeling of Resistive Plate Chambers, the most frequently used gas phase detectors of elementary particles in high energy experiments.
- Swarm studies provide best insight into non-hydrodynamic (or as plasma specialists call it non-local) development of the ionized gas. It is not only that simulations are simple but also some of the accurate experiments operate in such conditions and thus allow testing of such theories. One such example are the Franck Hertz oscillations. Temporal and spatial relaxation of properties of ensembles to the final distribution belong to this group as well and are of interest for a number of positron applications and trapping in general.
- Fluid models when applied to swarms provide a good way to test the fluid models as used in more general plasmas. This has yielded the need to generalize fluid equations and extend them to a one step further while using a higher order transport coefficients.
- Finally we shall address the open issues for transport theorists and atomic and molecular collision population in the attempt to represent transport of electrons, positrons and other particles in liquids, especially in water that has a strong dipole moment. Hydrated electrons and positrons are the actually particles of interest for modeling these particles in the human tissue.

As an interface between atomic and molecular collision physics on a lower phenomenological (but deeper) level and plasmas on a higher (but less fundamental) level swarm physics has the responsibility of providing plasma physics with its intellectual basis and fundamental importance. It is how we combine the building blocks of atomic and molecular physics, transport theory and other relevant elementary processes that will define generality of the conclusions about non-equilibrium plasmas that are all different and require a special approach.

The models that we provide here are simple, yet realistic and real systems that may be described by swarm models and that may be regarded as low ionization limits of some more complex non-equilibrium plasmas.

28th Summer School and International Symposium on the Physics of Ionized Gases

Aug. 29 - Sep. 2, 2016, Belgrade, Serbia

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Editors:
Dragana Marić, Aleksandar Milosavljević,
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MONTE CARLO SIMULATIONS OF ELECTRON TRANSPORT IN CF_3I AND SF_6 GASES

J. Mirić, D. Bošnjaković, I. Simonović, Z. Lj. Petrović and S. Dujko

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Pregrevica 118, 11080 Belgrade, Serbia

Abstract. Electron transport coefficients in CF_3I and SF_6 gases are calculated using Monte Carlo simulations for a wide range of reduced electric field strengths. In order to compensate for the loss of electrons in simulation due to strong attachment, three different rescaling techniques are considered and applied. Among many observed phenomena, in case of SF_6 we highlight the reduction of mean electron energy with increasing electric field. In addition, we observe that for both gases bulk drift velocities exhibit negative differential conductivity which is not present in the flux drift velocity.

1. INTRODUCTION

Electron attachment in strongly electronegative gases, such as CF_3I and SF_6, has many industrial applications. For example, in high-voltage circuit breakers, it is the most significant process for the prevention of electric breakdown [1]. Electronegative gases are also used for plasma etching and cleaning in semiconductor fabrication [2].

On the other hand, electron attachment imposes practical difficulties in experiments for measurement of transport coefficients [1,3]. Considerable difficulties also appear in Monte Carlo simulations of electron transport in strongly electronegative gases at low electric fields where electron attachment is the dominant process. Due to this process, the number of electrons in a simulation can reach extremely low values leading to poor statistics or complete loss of electrons in the simulation [4,5]. In order to compensate for this loss of electrons, some sort of rescaling techniques must be used.

In this work, we discuss the existing rescaling techniques for Monte Carlo simulations of electron transport in strongly electronegative gases. Furthermore, we introduce our modified rescaling procedure and demonstrate how these techniques affect the calculated transport data for CF_3I and SF_6 gases.

2. RESCALING TECHNIQUES

The following rescaling techniques, applicable for Monte Carlo simulations, can be found in the literature:

1. Duplication of electrons randomly chosen from the remaining swarm at certain discrete time steps [6];
2. Duplication of the entire electron swarm (one or more times) at certain time steps [5] or at certain distance steps [7];
3. Introduction of an additional fictitious ionization [4] or attachment process [8] with a constant collision frequency.

An unaltered electron distribution function and its evolution are a common objective for all these techniques. In this work, the first technique will be referred to as discrete rescaling, the second as swarm duplication and the third as continuous rescaling. However, we introduce a modification to the third procedure where the fictitious ionization process is dynamically adjusted during the simulation in such way that the fictitious ionization rate is chosen to be equal to the attachment rate. Therefore, it is not necessary to define a fictitious ionization rate in advance and as a benefit, the number of electrons is kept nearly constant during the simulation.

3. RESULTS

In this section, we present the transport data for CF_3I and SF_6 gases, calculated using our Monte Carlo code [6,9] with three different rescaling techniques. The cross section set for electron scattering in SF_6 is taken from Itoh *et al.* [10]. In case of CF_3I, we use our modified cross section set [11] which is based on cross sections of Kimura and Nakamura [12]. This modification of the CF_3I set was necessary in order to provide a better agreement between the calculated data and the reference data measured in a pulsed Townsend experiment for pure CF_3I and its mixtures with Ar and CO_2.

Figure 1(a) shows the variation of mean electron energy with E/n_0 in CF_3I. Calculations are performed assuming the three rescaling techniques. Excellent agreement between the cases of discrete rescaling and swarm duplication can be understood, having in mind that these two techniques are essentially the same. The only difference between the two is the fact that in case of discrete rescaling, the probability for duplication of an electron is determined by the ratio of current number and desired number of electrons, while in case of swarm duplication technique, this probability is set to unity i.e. the duplication is performed for all electrons. Continuous rescaling is also in a good agreement with the other two techniques.

In case of mean electron energy for the SF_6 gas, Figure 1(b) shows excellent agreement between the three rescaling techniques. Furthermore, one anomalous behavior is observed — a decrease of mean energy with increasing electric field. This phenomenon is associated with mutual influence of attachment heating and inelastic cooling. Since it is observed only in case of SF_6,

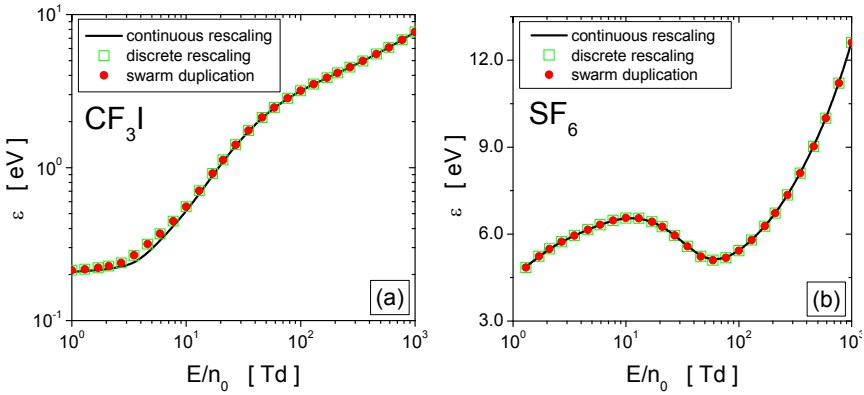

Figure 1. Mean electron energy in (a) CF_3I and (b) SF_6 gases as a function of reduced electric field. The profiles are calculated using three different rescaling techniques.

it is evident that the specific cross sections for electron scattering are essentially responsible for the occurrence of this phenomenon.

Figure 2 shows flux and bulk drift velocities in (a) CF_3I and (b) SF_6 gases, obtained with three rescaling techniques. For electrons in CF_3I, the drift velocities calculated using discrete rescaling and swarm duplication are again in excellent agreement while continuous rescaling at low electric fields gives slightly lower values than the other two techniques. For drift velocities in the SF_6 gas, all three rescaling techniques are in good agreement over the entire range of reduced electric fields considered in this work. We can conclude that the nature of the cross sections for electron scattering in CF_3I and SF_6 and their energy dependence are responsible for the differences between the results obtained using different rescaling techniques.

Two interesting phenomena are also observed in Figure 2. First, for

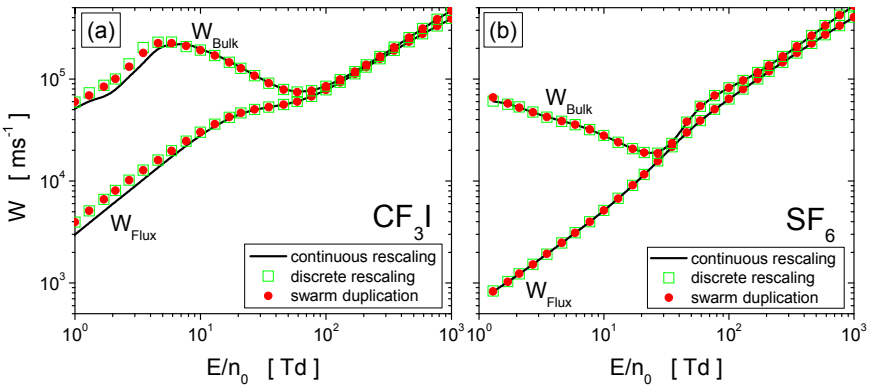

Figure 2. Variation of the drift velocity with E/n_0 for electrons in (a) CF_3I and (b) SF_6 gases. The profiles are calculated using three different rescaling techniques.

both gases the bulk drift velocity is higher than the flux drift velocity. In low energy range, this is a consequence of strong attachment heating (the consumption of slow electrons due to attachment) while in higher energy range the explicit effect of ionization is responsible. As a result, new electrons are preferentially created at the front of the swarm and/or slow electrons are consumed at the back of the swarm resulting in a forward shift of centre of mass of the swarm which is observed as an increase of bulk drift velocity over the flux drift velocity. The other phenomenon is a very strong NDC effect (negative differential conductivity) which is noticed for both gases, but only in case of bulk component drift velocity. This behavior appears to be common for all strongly electronegative gases since it is induced by explicit effects of electron attachment.

Acknowledgements

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ELECTRON TRANSPORT IN MERCURY VAPOR: DIMER INDUCED NDC AND ANALYSIS OF TRANSPORT PHENOMENA IN ELECTRIC AND MAGNETIC FIELDS

J. Mirić, I. Simonović, D. Bošnjaković, Z. Lj. Petrović and S. Dujko

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Abstract. Transport coefficients for electron swarms in mercury vapor in the presence of electric and magnetic fields are calculated and analyzed using a multi term theory for solving the Boltzmann equation and Monte Carlo simulation technique. Particular attention is paid to the occurrence of negative differential conductivity (NDC) at higher gas pressures and temperatures. It is shown that the correct representation of the presence of mercury dimers and superelastic collisions plays a key role in the analysis of NDC. When both the electric and magnetic fields are present, another phenomenon arises: for certain values of electric and magnetic field, we find regions where swarm mean energy increases with increasing magnetic field for a fixed electric field. Spatially-resolved electron transport properties are calculated using a Monte Carlo simulation technique in order to understand these phenomena.

1. INTRODUCTION

In this work we discuss the transport of electrons in mercury vapor and its mixtures with argon under conditions relevant for metal vapor lamps. Current models of such lamps require knowledge of transport coefficients as a function of electric field strengths, gas pressures and temperatures. Recently developed inductively coupled plasma light sources require the knowledge of transport coefficients when both the electric and magnetic fields are present and crossed at arbitrary angles [1]. These transport coefficients can be either measured in swarm experiments or calculated from transport theory. To date, no experiments exist that can measure all the required transport coefficients, including rate coefficients, drift velocities, and diffusion coefficients for electrons in gases in the presence of electric and magnetic fields.

In the present work we solve the Boltzmann equation for electron swarms undergoing ionization in mercury vapor and its mixtures with argon in the presence of electric and magnetic fields crossed at arbitrary angles. For the *E*-only case we discuss the occurrence of negative differential conductivity (NDC) for

higher gas pressures and temperatures in the limit of lower electric fields. NDC is a phenomenon where the drift velocity decreases with increasing electric field. For electrons in mercury vapor this behavior of the drift velocity is attributed to the presence of mercury dimers.

In the second part of this work we investigate the electron transport in varying configurations of electric and magnetic fields. In particular, we discuss the following phenomenon: for certain values of electric and magnetic fields, we find regions where swarm mean energy increases with increasing magnetic field for a fixed electric field. The phenomenon is discussed using spatially-resolved transport data calculated in Monte Carlo simulations.

2. CROSS SECTIONS AND SIMULATION TECHNIQUES

The cross section for momentum transfer in elastic collisions is made as follows. For lower electron energies, we use a cross section from [2] while for higher energies, we use a cross section tabulated in MAGBOLTZ code [3]. Cross sections for electronic excitations for levels $^3P_0$, $^3P_1$ and $^3P_2$ are retrieved from [4] while electronic excitations to $^1S_0$ and $^1P_1$ states as well as a cross section for higher states are also taken from MAGBOLTZ code. For electron-impact ionization, we have used a cross section from [5]. The effective cross section which describes vibration and electronic excitations of mercury dimers is derived using the experimental measurements of Elford [6]. Cross sections were slightly modified during the calculations to improve agreement between the calculated swarm parameters and the experimental values [6].

Electron transport coefficients are calculated from the multi term solution of Boltzmann's equation. A Monte Carlo simulation technique is used to verify the Boltzmann equation results and also for the calculations of spatially-resolved transport data.

3. RESULTS AND DISCUSSIONS

In Figure 1 (a) we show the variation of the drift velocity with E/n_0 for a range of gas pressures, as indicated on the graph. Calculations are performed in a wide range of pressures, from 20.2 to 108.4 Torr. The temperature of the background gas is 573K. The same range of pressures and temperatures was considered by Elford in his experiments [6]. We extend his measurements by considering the drift of electrons for six additional gas pressures. For E/n_0 less than approximately 2.5 Td the pressure dependence of the drift velocity is clearly evident. For higher E/n_0, however, the drift velocity does not depend on the pressure. For pressures higher than approximately 200 Torr, we see that the drift velocity exhibits a region of NDC, i.e. over a range of E/n_0 values the drift velocity decreases as the driving field is increased. The conditions for the occurrence of NDC have been investigated previously [7]. For electrons in mercury vapor, NDC arises for certain combinations of elastic cross sections of dimer-free mercury vapor and inelastic cross sections of mercury dimers in

which, on increasing the electric field, there is a rapid transition in the dominant energy loss mechanism from inelastic to elastic. For pressures lower than 200 Torr the elastic cross section of dimer-free mercury vapor dominates the effective inelastic cross section of mercury dimers. Thus, the conditions for the occurrence of NDC are not set. For higher pressures, the phenomenon is promoted by either or both of (i) a rapidly increasing cross section for elastic collisions and (ii) a rapidly decreasing inelastic cross section. It is clear that the presence of dimmers plays a key role in the development of NDC in mercury vapor.

In Figure 1 (b) we show a comparison between our calculations and experimental measurements of the drift velocity for a range of pressures. Our Monte Carlo results (figure 1 (b)) agree very well with those measured in the Bradbury-Nielsen time-of-flight experiment [6]. The agreement is achieved only after careful implementation of superelastic collisions in our calculations. Cross sections for superelastic collisions are calculated directly in our code from the principle of detailed balance.

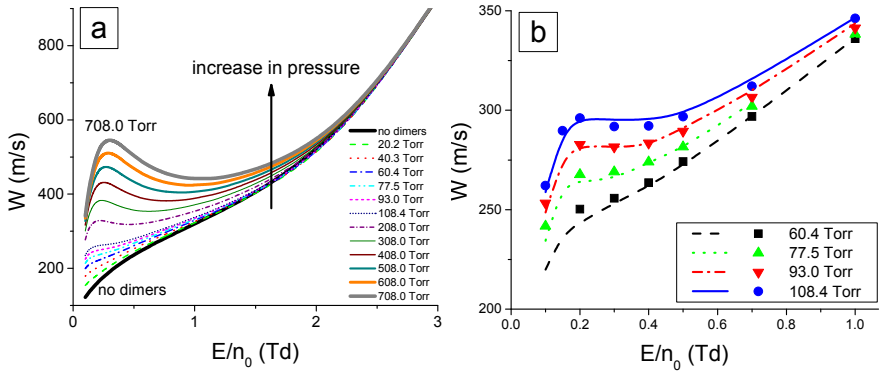

Figure 1. Variation of the drift velocity with E/n_0 for a range of pressures (a) and comparison between our Monte Carlo results and experimental measurements. Calculations are performed for electrons in mercury vapor. The temperature of the background gas is 573K.

In the last segment of this work we discuss the impact of a magnetic field on the electron transport in mercury vapor. The pressure and temperature of the mercury vapor are set to 1 Torr and 293K, respectively. As an example of our study, in figure 2 we show the variation of the mean energy with E/n_0 for a range of the reduced magnetic fields B/n_0, in a crossed field configuration. In the limit of the lowest E/n_0 the electrons are essentially in the quasi-thermal equilibrium with the mercury vapor, independent of the strength of the applied magnetic field. In this regime, the longitudinal and transverse drift velocity components are dependent on both E/n_0 and B/n_0 while the diagonal diffusion tensor elements along the **E** and **E**×**B** directions are dependent on B/n_0 only. The diffusion coefficient along the magnetic field direction is reduced to its thermal value as magnetic field only affects the diffusion in this direction indirectly, through the magnetic field's action to cool the swarm. Certainly one of the most striking

properties observed in the profiles of transport coefficients is an increase in the swarm mean energy with increasing magnetic field for a fixed electric field. The phenomenon is evident in the range E/n_0=5-200 Td for B/n_0 considered in this work. This behavior is contrary to previous experiences in swarm physics as one would expect the mean swarm energy to decrease with increasing B/n_0 for a fixed E/n_0. The phenomenon could be associated with the interplay between magnetic field cooling and inelastic/ionization cooling, although the role of the cross sections in both phenomena is of course vital. The electron energy distribution function and spatially-resolved mean energy, rate coefficients and other properties are calculated using a Monte Carlo simulation technique in order to explain this phenomenon.

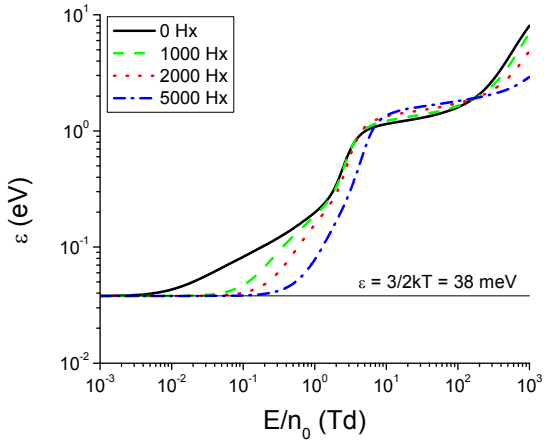

Figure 2. Variation of the mean energy with E/n_0 for a range of B/n_0. Calculations are performed for electrons in mercury vapor.

Acknowledgements

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SCATTERING CROSS SECTIONS AND TRANSPORT COEFFICIENTS FOR ELECTRONS IN CF_3I

J. Mirić[1], O. Šašić[1,2], S. Dujko[1] and Z.Lj. Petrović[1]

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Abstract. Scattering cross sections for electrons in CF_3I are discussed using the swarm method. Electron drift velocity, effective ionization coefficient and diffusion coefficients are calculated using a Monte Carlo simulation technique and from solution of the non-conservative Boltzmann equation. Calculated data for pure CF_3I and its mixtures with rare gases, N_2 and SF_6 are compared with those measured experimentally under both the time-of-flight and pulsed-Townsend conditions. Among many important phenomena observed in electron transport we note the existence of negative differential conductivity in the profile of the bulk drift velocity with no signs of the same phenomenon in the profile of flux drift velocity.

1. INTRODUCTION

Trifluoroiodomethane (CF_3I) is a processing gas employed for plasma etching of various materials. Due to its short atmospheric lifetime (1.8 days), low GWP (0.4 times than of CO_2) and high critical electric field (437 Td) CF_3I shows a promise for application as an alternative refrigerant to commonly used fluorocarbons such as CF_4 [1], and as a potential high voltage insulator, both on its own and mixed with N_2 and CO_2 in high-voltage insulation technology [2]. In spite of these important applications of CF_3I, still there is a lack of reliable sets of cross sections for electron scattering and associated electron transport coefficients.

In this work we discuss the existing sets of cross sections for electron scattering in CF_3I. Using the swarm method, our initial set of cross sections is constructed from other available sets, and data for individual scattering channels. Calculated transport data are then compared with those measured in experiments and if the agreement is not enough, then cross sections are modified. This process is repeated until some preset agreement between theoretically calculated and experimentally measured data is achieved. Increasing the accuracy of the set of

cross sections, the electron transport is investigated using the multi term approach for solving the Boltzmann equation where particular emphasis was placed upon the explicit effects of non-conservative collisions on the drift and diffusion.

2. CROSS SECTIONS FOR ELECTRON SCATTERING IN CF_3I

The initial set of cross sections in this work was developed by Kimura and Nakamura [3], and is presented by solid curves in Figure 1. Due to disagreement between experimentally measured swarm data and those obtained in theoretical calculations, we have concluded that there are some internal inconsistencies in the set proposed by Kimura and Nakamura. Similar conclusions have been recently found by Kawaguchi *et al.* [4].

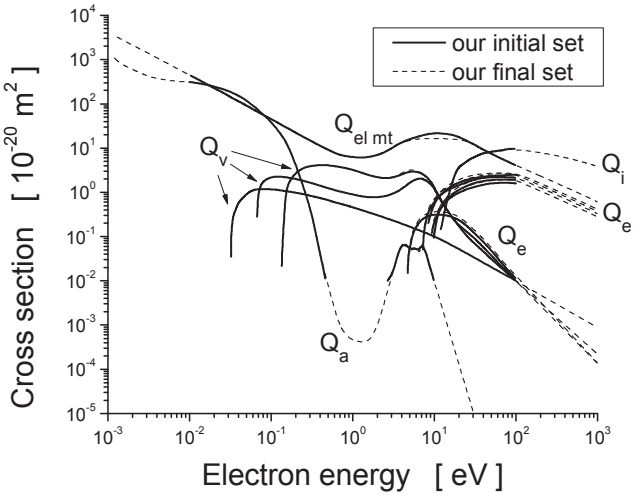

Figure 1. Cross sections for electron scattering in CF_3I from Kimura and Nakamura (solid curves) [3] and from our work (broken curves).

In this work the cross sections were extended in energy up to 1000 eV so that calculated data may cover the region between a few Td and few thousands of Td. This is of great importance having in mind the high critical field of CF_3I. The logarithmic extrapolation was used for electronic excitation with the lowest threshold and for all vibrational excitations as well as for the electron attachment. The Born-Bethe approximation was used to extrapolate the cross sections for momentum transfer in elastic collisions and for the cross sections for electronic excitation. The cross section for ionization was modified as follows: in the energy range up to 45 eV we have used the cross section from [3] while for higher energies than 45 eV we have included the theoretically calculated cross section developed by Anthony *et al.* [5]. Using the data

suggested by Christophorou [6], the cross section for attachment between 0.5 and 3 eV was reconstructed.

Cross section for momentum transfer in elastic collisions in the energy region between 4 and 20 eV was modified together with the cross section for vibrational excitation with the highest threshold in order to fit the drift velocity from experimental measurements of Kimura and Nakamura [3]. The ionization coefficient was fitted through the modification of cross sections for electronic excitations having in mind the large uncertainties associated with the magnitudes of these cross sections. Our final set of cross sections for electron scattering in CF_3I is shown in Figure 1. This set of cross sections provides much better agreement between theoretically calculated and experimentally measured swarm transport data as discussed below.

3. TRANSPORT COEFFICIENTS FOR ELECTRONS IN CF_3I

In Figure 2 we compare our results for the electron drift velocity with experimental data obtained under the time-of-flight [3] and pulsed-Townsend conditions [2]. The calculated values of W are initially lower than those measured in experiments. After modification of cross sections the calculated values of W are in a good agreement with experimental measurements obtained under the time-of-flight conditions. Our flux drift velocity is calculated by the two-term approximation (TTA) for solving the Boltzmann equation and using a Monte Carlo simulation technique.

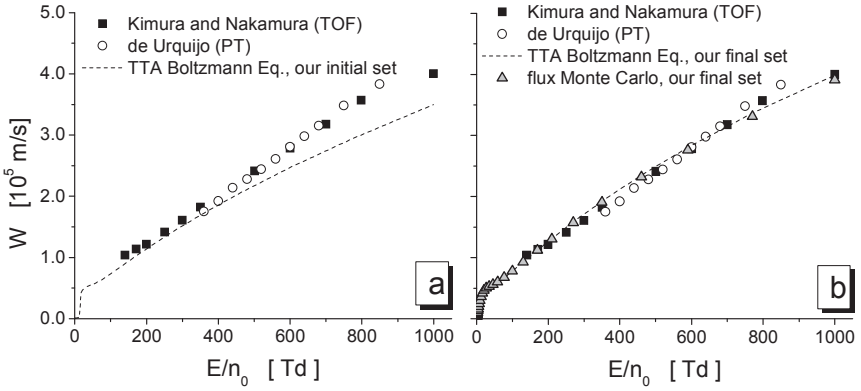

Figure 2. Variation of the drift velocity with E/n_0 for electrons in CF_3I. Our TTA results are compared with those obtained in experiments for (a) our initial set of cross sections and (b) our final set of cross sections.

Figure 3 shows the calculated values of effective ionization coefficient $(\alpha\text{-}\eta)/n_0$ using the initial set of cross sections (a) and our final set of cross sections (b). Values of $(\alpha\text{-}\eta)/n_0$ measured by Kimura and Nakamura [3] and de

Urquijo *et al.* [2] are also plotted. In Figure 3 (a), calculated values of $(\alpha-\eta)/n_0$ are higher than the measured data for higher E/n_0. Calculated values using our final set of cross sections agree well with the measured data in a wide range of E/n_0 except for E/n_0 less than approximately 200 Td where the effects of attachment are dominant.

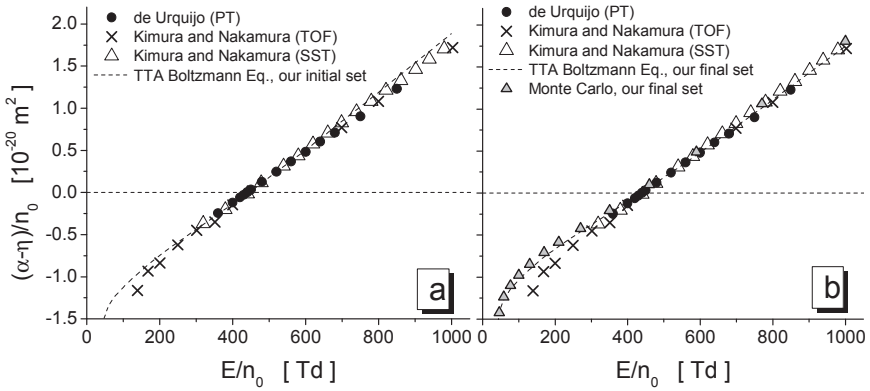

Figure 3. Variation of the effective ionization coefficient with E/n_0 for electrons in CF_3I. Our TTA results are compared with those obtained in experiments for (a) our initial set of cross sections and (b) our final set of cross sections.

Other transport properties including diagonal elements of the diffusion tensor, mean energy and rate coefficients are also calculated using a Monte Carlo simulation technique and from multi term solutions of the Boltzmann equation. Bulk values of the drift velocity and diffusion coefficients are evaluated and explicit effects of the electron attachment and/or ionization are examined.

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ELECTRON TRANSPORT IN NOBLE-GAS METAL-VAPOR MIXTURES

J. Mirić[1], Z.Lj. Petrović[1], R.D. White[2] and S. Dujko[1]

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Abstract. Electron transport coefficients required for the modeling of light sources are calculated from the multi term solution of the non-conservative Boltzmann equation. Calculations are performed over a range of E/n_0 values (ratio of the electric field, E, to the neutral number density n_0), gas temperatures and metal vapor concentrations relevant to lamp discharges. Values and general trends of mean energy, drift velocity, diffusion tensor and rate coefficients are presented in this work.

1. INTRODUCTION

The progress and further improvements of light sources based on low or high pressure electrical gas discharges require the most accurate modeling of charged particle transport processes in noble-gas-metal-vapor mixtures [1]. In particular, modern high intensity discharge lamps are usually filled with noble gas at high pressure (0.1 to 12 bar) and metallic salts. Noble gas provides light during the initial warm-up phase of the operation while metallic salts take over light emission after they have evaporated [2]. Our work has been motivated, in part, by recent suggestions that highly accurate data for transport coefficients required as input in fluid models of lamp discharges may significantly improve the existing models. Current models of such lamps require knowledge of the plasma electrical conductivity, which can be calculated from the cross sections for electron scattering in noble-gas-metal-vapor mixtures and mobility coefficients presented in this work.

In this work we investigate electron transport in mixtures of noble gases (He, Ne, Ar, Kr and Xe) and metal vapors (Na, K, Cs, Mg and Hg)

under swarm conditions using a multi term theory for solving the Boltzmann equation [3]. In section 2, we give a brief discussion of the theoretical multi term solution of the Boltzmann equation under non-conservative conditions while in section 3 we present a few examples of our systematic study of electron transport in noble-gas-metal-vapor mixtures.

2.THEORETICAL METHODS

Electron transport coefficients are determined by solving the non-conservative Boltzmann's equation under the hydrodynamic conditions for electrons drifting and diffusing through the noble-gas-metal-vapor mixtures under the influence of spatially homogeneous electric field. In brief, the solution of Boltzmann's equation is found be expanding the distribution function as sums of products with the directional dependence of $\boldsymbol{c}$ contained in spherical harmonics $Y_l^{(m)}(\hat{\boldsymbol{c}})$ (where $\boldsymbol{c}$ is the electron velocity), the spatial distribution contained in $G_\mu^{(s\lambda)}$, the s-th application of the spatial gradient operator operating on $n(\boldsymbol{r},t)$, and the speed distribution contained in an expansion discussed below [3]. Thus, we have

$$f(\boldsymbol{r},\boldsymbol{c},t)=\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\sum_{s=0}^{\infty}\sum_{\lambda=0}^{s}\sum_{\mu=-\lambda}^{\lambda} f\left(lm|s\lambda\mu\right)Y_l^{(m)}(\hat{\boldsymbol{c}})G_\mu^{(s\lambda)}n(\boldsymbol{r},t). \qquad (1)$$

The coefficients $f\left(lm|s\lambda\mu\right)$ are functions of the speed c and are obtained by the expansion

$$f\left(lm|s\lambda\mu\right)=\omega\left(T_b,c\right)\sum_{\nu=0}^{\infty}F\left(\nu lm|s\lambda\mu\right)R_{\nu l}\left(T_b,c\right), \qquad (2)$$

where $\omega\left(T_b,c\right)$ is a Maxwellian distribution at a temperature T_b. T_b is not equal to the neutral gas temperature and serves as an adjustable parameter to optimize the convergence. $R_{\nu l}$ are related to a Sonnine polynomial of order (ν,l) while the coefficients $F\left(\nu lm|s\lambda\mu\right)$ are the so-called moments that are relatively simply related to transport coefficients. The classical two term approximation (TTA) for solving the Boltzmann equation covers only the range in l of 0 and 1, which is not sufficient for good accuracy in noble-gas metal-vapors. Using the above decomposition of f (1), the Boltzmann equation is converted to a hierarchy of doubly infinite set of coupled algebraic equations for the moments. The resulting coefficient matrix is sparse and direct numerical inversion procedure is used to calculate the moments.

3.RESULTS AND DISCUSSIONS

The transport coefficients shown below are functions of E/n_0 and are expressed using the unit townsend (1 Td= $10^{-21}\mathrm{Vm}^{-1}$). In this work

we will cover a range of E/n_0 up to 1000 Td. The temperature of Hg vapor is varied between 0 and 8000 K. The internal states are assumed to be governed by a Maxwell-Boltzmann distribution which essentially places all metal-vapor atoms in the ground state for the temperatures considered. The effects of dimmers are not included. Cross sections for electron scattering in Na, K and Cs are taken from [4] while for Hg and Mg are taken from the Lxcat database [5].

In figure 1 (a) we show the variation of the mean energy with E/n_0 and gas temperature T, for electrons in Hg vapor. For lower E/n_0 the mean energy is different for different gas temperatures and only for $T = 8000$ K the electrons are in thermal equilibrium with the Hg vapor. This means that the electron velocity distribution is approximately thermal-Maxwellian. For increasing E/n_0 the effects of the gas temperature are less pronounced; the electron velocity distribution is non-equilibrium and non-Maxwellian though transport properties are still dependent on T. In the limit of higher E/n_0, the electron swarm is far from thermal-equilibrium and the influence of the Hg vapor temperature can be neglected.

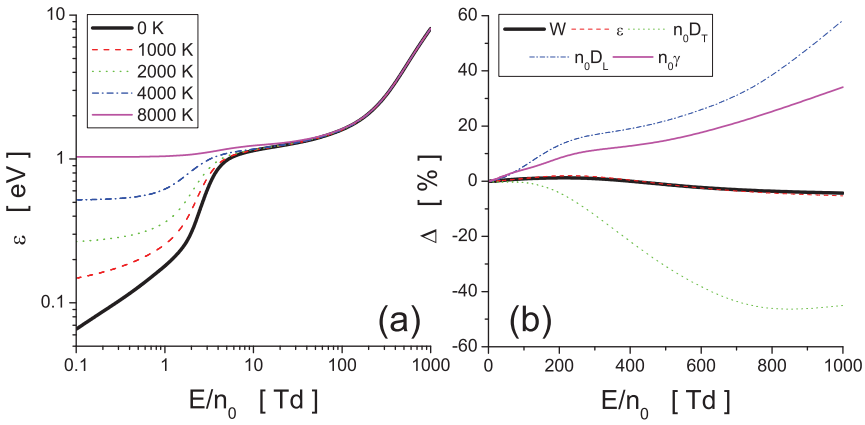

Figure 1. (a) Variation of the mean energy with E/n_0 and gas temperature T for electrons in Hg vapor. (b) Percentage difference between the two term and multi term results for various transport properties. The gas temperature is set to 293 K.

In figure 1 (b) we illustrate the errors associated with the TTA for solving the Boltzmann equation for electrons in Hg vapor. We observe that increasing E/n_0 deteriorates the accuracy of the TTA. For the chosen set of conditions, the mean energy and drift velocity have the errors of the order of 5% while the errors of the diffusion coefficients are much higher and are of the order of 50 %.

Figure 2 (a) shows the variation of the mean energy and drift ve-

locity with E/n_0 for electrons in various metal-vapors. For lower E/n_0, we observe that the electrons are in thermal-equilibrium only with the K-vapor. The properties of the cross sections are reflected in the profiles of the mean energies. When elastic collisions are dominant, the mean energy grows very fast. Much slower rise of the mean energy is a consequence of the large energy loss of the electrons as the inelastic channels become important. Except for very low E/n_0 the mean energy in Hg vapor dominates the mean energies of electrons in other vapors.

From figure 2 (b) we see that for $E/n_0 \geq 6$ Td the drift velocity in Hg vapor dominates the drift velocities of electrons in other vapors. This suggests that plasma electrical conductivity will be the highest for Hg vapor.

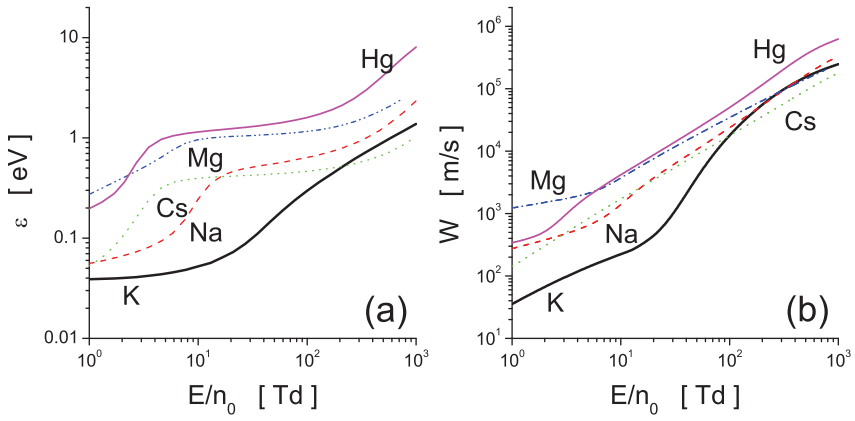

Figure 2. Variation of the mean energy (a) and drift velocity (b) with E/n_0 for electrons in metal-vapors. The gas temperature is $T = 298$ K.

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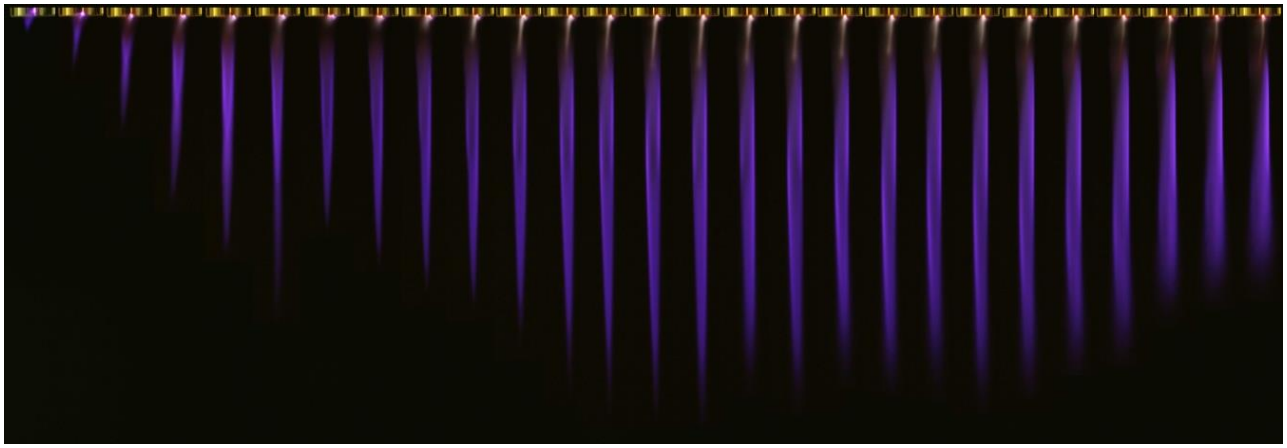

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Scattering cross sections and transport data for electrons in CF_3I

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The trifluoroiodomethane (CF_3I) is a halofluorocarbon gas employed in the plasma etching of various materials. It also shows promise as a gaseous dielectric in the application of high-voltage power equipment. This is an environmentally friendly gas due to the following characteristics. First, C-I bond in this molecule is weak so can easily be broken by ultraviolet light which leads to a very short atmospheric lifetime (1.8 days). GWP (global warming potential) of CF_3I is ultra low (0.4 times that of CO_2) [1]. Second, this molecule has higher critical electric field (437 Td) [2] than SF_6 and hence it meets the basic requirements for application to environmentally-benign power equipment. Despite the need for reliable swarm and cross section data, there have only been a few swarm measurements of transport data covering relatively narrow *E/N* range [2] and only one set of cross sections for electron scattering [3]. This work represents an attempt to overcome such lack of reliable collisional and transport data for CF_3I.

Cross sections for electron scattering are critical input data in modeling of plasma discharges. The compilation of the cross-sections from different sources, without their renormalization to fit the swarm parameters, is usually not sufficient. Starting from the existing set of cross sections for electrons in CF_3I [3], we have employed a standard swarm procedure for the analysis of measured drift velocities and effective ionization coefficient.

In [3] the momentum transfer is composed of theoretical values up to 0.5 eV by Christophorou [4] while in the energy range between 1.5 and 60 eV the numerical integration of the differential cross sections of Kitajima [5] was performed. For higher energies the momentum transfer cross section is found as a sum of individual cross sections for momentum transfer of constituent atoms [6, 7]. The attachment cross section suggested by Christophorou [4] was included and six vibrational modes of CF_3I by Shimanouchi [8] were grouped into three. The total ionization cross section is given as a sum of experimentally determined partial ionization cross sections [9]. Finally, in the same set of cross sections there are five cross sections for electronic excitations (and possibly neutral dissociation) whose magnitudes were decided by considering the relative loss peak height of Kitajima [5]. Using a two-term Boltzmann code, the calculated transport coefficients (drift velocity under the time-of-flight conditions and rate coefficients for ionization and attachment obtained under the steady-state Townsend conditions) were compared with the corresponding experimental data and in figure 1(a) we show the final set of cross sections developed by Kimura and Nakamura [3]. This is the initial set of cross sections used in this work.

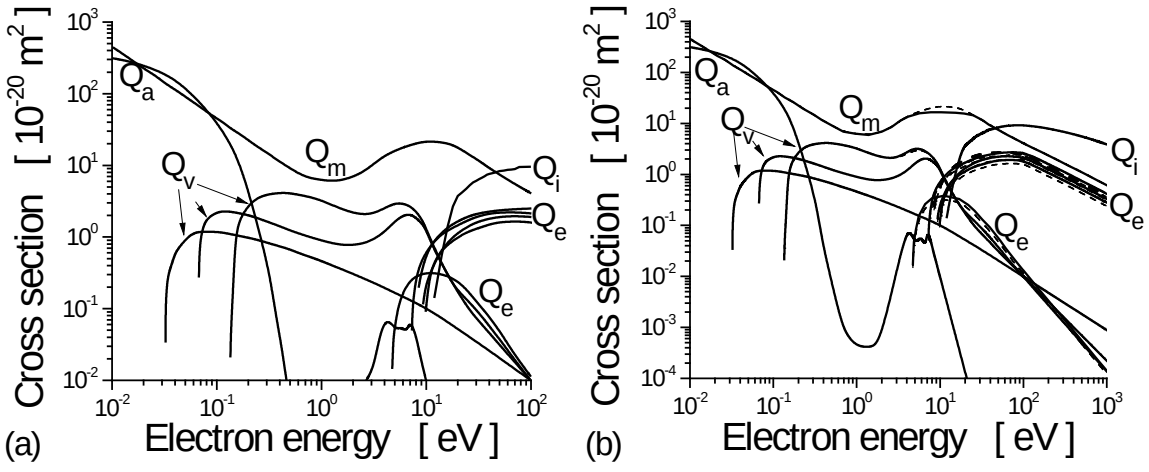

Figure 1. Cross section sets for electron scattering of CF_3I: (a) from Kimura and Nakamura's work [3], (b) from this work (solid curves - our final and dashed curves - our initial set of cross sections).

The first step in our work was calculation of transport data based on the cross sections developed in [3]. Calculations of transport coefficients were performed by Bolsig+ [10] and our Monte Carlo simulation code and the results for the drift velocity and rate coefficients for attachment and ionization were compared with the available experimental measurements. The disagreement between these two sets of data was an indication of some internal inconsistencies within the set of cross sections developed by Kimura and Nakamura [3].

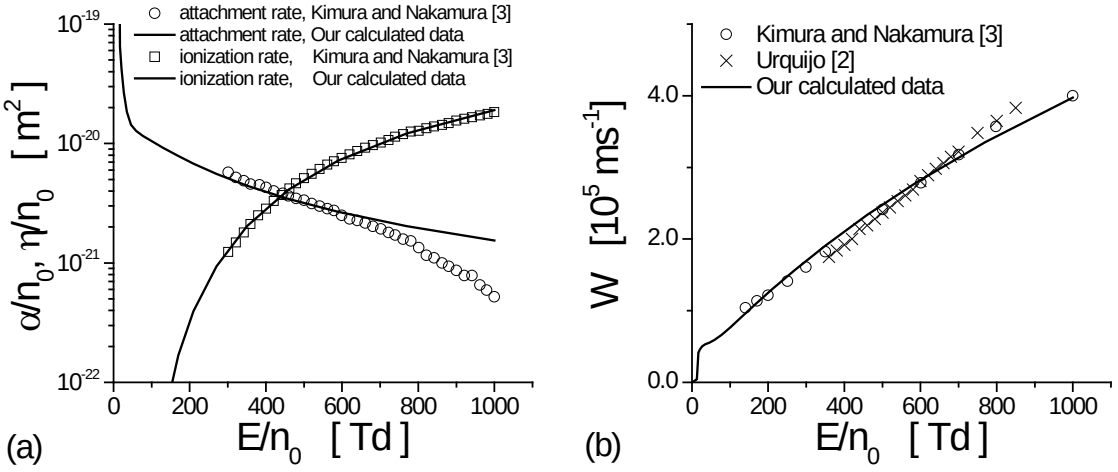

Figure 2. Comparison of our calculated and experimentally measured transport coefficients presented [2,3]: (a) ionization and attachment rates, and (b) drift velocity.

In this work the cross-sections were extended in energy up to 1000 eV so that calculated data may cover the region between a few Td and few thousands of Td. This is of great importance having in mind the high critical field of CF_3I. The logarithmic extrapolation was used for electronic excitation with the lowest threshold and for all vibrational excitations as well as for the electron attachment. The Born-Bethe approximation was used to extrapolate the cross sections for momentum transfer in elastic collisions and for the cross sections for electronic excitation. The cross section for ionization was modified as follows: in the energy range up to 45 eV we have used the cross section from [3] while for higher energies than 45 eV we have included the theoretically calculated cross section developed by Anthony [11]. Using the data suggested by Christophorou

[4], the cross section for attachment between 0.5 and 3 eV was reconstructed.

Cross section for momentum transfer in elastic collisions in the energy region between 4 and 20 eV was modified together with the cross section for vibrational excitation with the highest threshold in order to fit the drift velocity from experimental measurements of Kimura and Nakamura [3]. The ionization coefficient was fitted through the modification of cross sections for electronic excitations having in mind the large uncertainties associated with the magnitudes of these cross sections. Our cross sections for electron scattering in CF_3I are shown in figure 1(b). This set of cross sections provides much better agreement between theoretically calculated and experimentally measured swarm transport data as shown in figure 2.

In this work the cross section set for electron-CF_3I collisions was developed on the basis of the cross sections developed by Kimura and Nakamura [3]. Further improvements of the present set will be made by considering the transport data in the mixtures of CF_3I with Ar, Xe and N_2.

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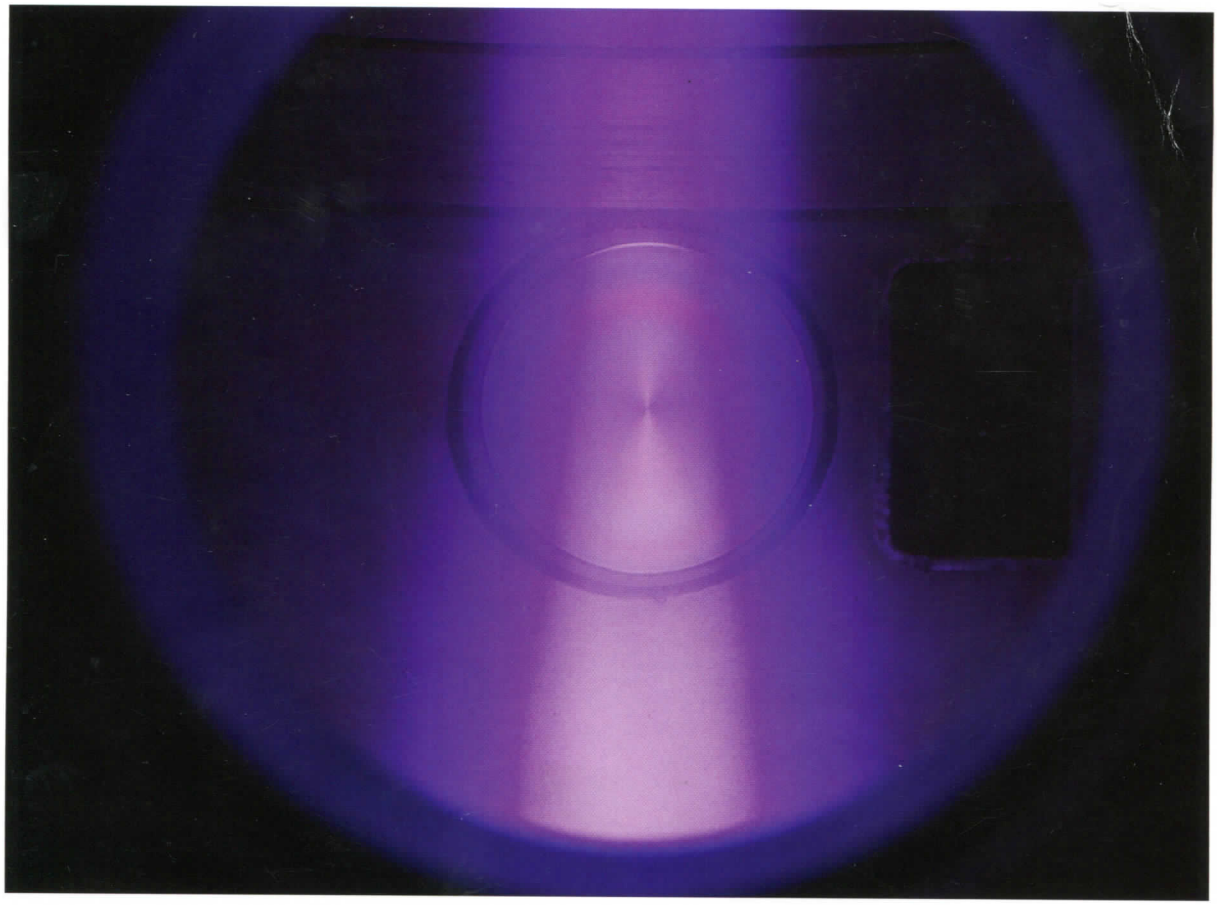

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coefficients for low and moderate reduced electric fields E/N (N-gas density) accounting for non-conservative processes.

*Acknowledgment to Ministry of Education, Science and Technology of Republic Serbia, Projects No. 171037 and 410011.

MW6 35 Third order transport coefficients for electrons and positrons in gases SASA DUJKO, ILIJA SIMONOVIC, *Institute of Physics, University of Belgrade, Serbia* RONALD WHITE, *College of Science, Technology & Engineering, James Cook University, Australia* ZORAN PETROVIC, *Institute of Physics, University of Belgrade, Serbia* Third order transport coefficients (the skewness tensor) of the electron and positron swarms, in atomic and molecular gases, are investigated. The knowledge of the skewness tensor is necessary for the conversion of the hydrodynamic transport coefficients to the arrival time and steady-state Townsend transport data as well as for the determination of the deviations of the spatial density profiles from an ideal Gaussian. In this work, we investigate the structure and symmetries along individual elements of the skewness tensor by the group projector method. Individual components of the skewness tensor are calculated using a Monte Carlo simulation technique and multi term theory for solving the Boltzmann equation. Results obtained by these two methods are in excellent agreement. We extend previous studies by considering the sensitivity of the skewness components to explicit and implicit effects of non-conservative collisions, post-ionization energy partitioning, and inelastic collisions. The errors of the two term approximation for solving the Boltzmann equation are highlighted. We also investigate the influence of a magnetic field on the skewness tensor in varying configurations of electric and magnetic fields. Among many interesting points, we have observed a strong correlation between the skewness and diffusion.

MW6 36 Transport properties of electrons and transition of an electron avalanche into a streamer in atomic liquids SASA DUJKO, ILIJA SIMONOVIC, *Institute of Physics, University of Belgrade, Serbia* GREGORY BOYLE, RONALD WHITE, *College of Science, Technology & Engineering, James Cook University, Australia* DANKO BOSNJAKOVIC, ZORAN PETROVIC, *Institute of Physics, University of Belgrade, Serbia* A Monte Carlo simulation technique is developed and used to calculate transport coefficients of electron swarms in non-polar atomic liquids. We employ the two model processes in which only momentum and energy are exchanged, respectively, to account for structure dependent coherent elastic scattering at low energies. The validity of the code is confirmed by comparison with results of previous authors. We apply two scenarios for higher energy cross sections. In the first scenario excitations in the liquid phase are approximated by excitations in the gas phase. In the second scenario excitations are completely neglected. Ionization threshold is reduced to values which are suggested in the literature, in both scenarios. Transport coefficients in these two scenarios, as well as transport coefficients for gas and liquid phases are compared. Special attention has been given to the structure induced negative differential conductivity (NDC), which has been observed both in this work, and in previous publications. Spatially-resolved electron transport properties are calculated in order to understand this phenomenon. The important aspect of this work is modeling of the transition of an electron avalanche into a streamer. Calculations are performed using 1D and 1.5D fluid models. Streamer properties in scenarios with and without excitations are compared.

MW6 37 Monte Carlo simulations of electron transport in strongly attaching gases ZORAN PETROVIC, JASMINA MIRIC, ILIJA SIMONOVIC, DANKO BOSNJAKOVIC, SASA DUJKO, *Institute of Physics, University of Belgrade, Serbia* Extensive loss of electrons in strongly attaching gases imposes significant difficulties in Monte Carlo simulations at low electric field strengths. In order to compensate for such losses, some kind of rescaling procedures must be used. In this work, we discuss two rescaling procedures for Monte Carlo simulations of electron transport in strongly attaching gases: (1) discrete rescaling, and (2) continuous rescaling. The discrete rescaling procedure is based on duplication of electrons randomly chosen from the remaining swarm at certain discrete time steps. The continuous rescaling procedure employs a dynamically defined fictitious ionization process with the constant collision frequency chosen to be equal to the attachment collision frequency. These procedures should not in any way modify the distribution function. Monte Carlo calculations of transport coefficients for electrons in SF_6 and CF_3I are performed in a wide range of electric field strengths. However, special emphasis is placed upon the analysis of transport phenomena in the limit of lower electric fields where the transport properties are strongly affected by electron attachment. Two important phenomena arise: (1) the reduction of the mean energy with increasing E/N for electrons in SF6, and (2) the occurrence of negative differential conductivity in the bulk drift velocity of electrons in both SF_6 and CF_3I.

MW6 38 Electron transport in mercury vapor: magnetic field effects, dimer induced NDC and multi-term analysis ZORAN PETROVIC, JASMINA MIRIC, ILIJA SIMONOVIC, SASA DUJKO, *Institute of Physics, University of Belgrade, Serbia* A multi term theory for solving the Boltzmann equation and Monte Carlo simulation technique are used to investigate electron transport in varying configurations of electric and magnetic fields in mercury vapor. Using different sets of cross sections for electron scattering in mercury as an input in our Boltzmann and Monte Carlo codes, we have calculated data for electron transport as a function of reduced electric and magnetic fields. A multitude of kinetic phenomena in electron transport has been observed and discussed using physical arguments. In particular, we discuss two important phenomena: (1) for certain values of electric and magnetic field, we find regions where swarm mean energy increases with increasing magnetic field for a fixed electric field, and (2) the occurrence of negative differential conductivity (NDC) for higher pressures and temperatures. In particular, NDC is induced by the presence of mercury dimers. The measured drift velocities agree very well with our Monte Carlo results only if the superelastic collisions are included in our calculations. Spatially-resolved electron transport properties are calculated using a Monte Carlo simulation technique in order to understand these phenomena.

MW6 39 Dependence of ion drift velocity and diffusion coefficient in parent gas on its temperature* SERGEY MAIOROV, *Joint Institute for High Temperatures of RAS, Moscow* RUSUDAN GOLYATINA, *A.M. Prokhorov General Physics Institute of RAS, Moscow* The results of Monte Carlo calculations of the ion drift characteristics are presented: ions of noble gases and Ti, Fe, Co, Cs, Rb, W and mercury ions in case of constant and uniform electric field are considered. The dependences of the ion mobility on the field strength and gas temperature are analyzed. The parameters of the drift velocity approximation by the Frost formula for gas temperatures of 4.2, 77, 300, 1000, and 2000 K are presented. A universal drift velocity approximation depending on the reduced electric field strength and gas temperature is obtained. In the case of strong electric fields or low gas temperatures, the deviation of the ion distribution function from the Maxwellian one (including the shifted Maxwellian one) can be very significant. The average

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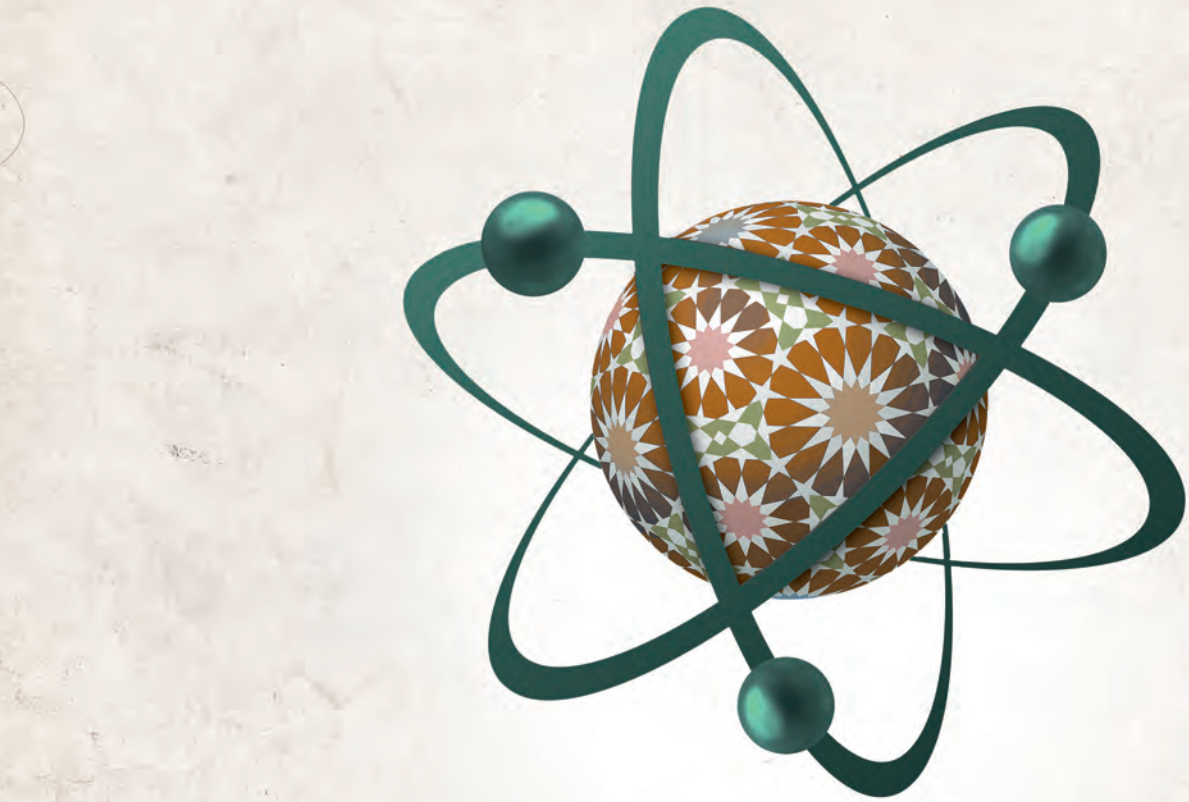

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E-02

Rescaling procedures for Monte Carlo simulations of electron transport in strong electronegative gases

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Electron attachment often imposes practical difficulties in Monte Carlo (MC) simulations of electron transport in strong electronegative gases at low electric field strengths. If the attachment rate is too high, the entire electron swarm can be consumed before steady state is achieved. In such extreme cases the transport data cannot be calculated. An obvious solution would be to use a very large number of initial electrons. However, in order to obtain the results with reasonable statistical accuracy, this would usually require computing resources which are beyond practical limits.

In order to address this issue in an optimal fashion, two distinctive procedures for electron compensation were proposed. The first one, which we refer to as *discrete rescaling*, is based on duplication of electrons randomly chosen from the remaining swarm at certain discrete time instants [1]. The other one we refer to as *continuous rescaling* introduces a fictitious ionization process with constant collision frequency chosen to be roughly equal to the attachment rate [2]. Both of these procedures were devised with the aim not to alter the electron distribution function and its evolution. However, it can be shown theoretically that only continuous rescaling meets this requirement [2].

In this work, we investigate the effects of MC rescaling procedures on the electron transport in CF_3I and SF_6 gases. Additionally, we propose a new implementation of continuous rescaling procedure which does not require the fictitious ionization rate to be defined *a priori*. Transport data is calculated using our electron impact cross sections for CF_3I [3] and a cross section set for SF_6 developed by Itoh et al. (1993). The results show that in case of CF_3I the transport parameters obtained using these two rescaling procedures can differ as much as 30% for the flux drift velocity or the attachment rate. Figure 1 shows the calculated flux drift velocity for CF_3I over a range of reduced electric field strengths. The results calculated using two term approximation for solving Boltzmann equation (BE TTA), are also shown for comparison.

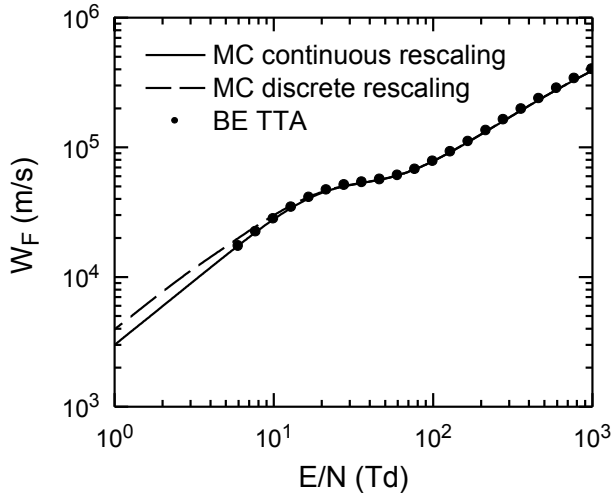

Figure 1. Flux drift velocity for CF_3I calculated over a range of reduced electric field strengths using two different MC rescaling procedures. Values obtained using two term approximation for solving Boltzmann equation are also shown (BE TTA).

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SCATTERING CROSS SECTIONS AND ELECTRON TRANSPORT COEFFICIENTS FOR ELECTRONS IN CF_3I

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Electron transport coefficients and rate coefficients in pure CF_3I and its mixtures with Ar, Xe, N_2 and SF_6 have been calculated for a set of cross-sections which was based on the work of Kimura and Nakamura [1] but which was modified to improve agreement between the calculated swarm parameters and the experimental values. Electron drift velocity, effective ionization coefficient and diffusion coefficients are calculated using a Monte Carlo simulation technique and from solution of the non-conservative Boltzmann equation [2]. Calculated data for pure CF_3I and its mixtures with Ar, Xe, N_2 and SF_6 are compared with those measured under both time-of-flight (TOF) and pulsed-Townsend (PT) conditions. We note the existence of negative differential conductivity (NDC) in the profile of the bulk drift velocity with no signs of the same phenomenon in the profile of flux drift velocity. We systematically study the origin and mechanisms for such phenomena as well as the possible physical implications which arise from their explicit inclusion into plasma models. Spatially-resolved electron transport properties are calculated using a Monte Carlo simulation technique in order to understand these phenomena. Special attention is paid upon the implementation of procedure for compensation of electrons for losses due to strong electron attachment in our Monte Carlo code.

The Monte Carlo method is used to analyze the behavior of electron transport coefficients in radio-frequency electric field in pure CF_3I. Among many interesting kinetic phenomena, we observe the time-resolved NDC and anomalous anisotropic behavior of the longitudinal diffusion coefficient. We explore the validity of the quasi-static approximation for lower field frequencies and effective field approximation for higher frequency for electrons in CF_3I.

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XVIII International Symposium on Electron-Molecule Collisions and Swarms

Programme and Book of Abstracts

XVII International Workshop on Low-Energy Positron and Positronium Physics &
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19 - 21 July 2013, Kanazawa, Japan

POSMOL 2013

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POSMOL 2013

Abstracts of Plenary Talks

Abstracts of Progress Reports (ems)

TE-06

Non-conservative electron transport in gases and its application in modelling of non-equilibrium plasmas and particle detectors

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The advancements in modern day technology associated with non-equilibrium plasma discharges depend critically on accurate modeling of the underlying collision and transport processes of charged particles in gases. To meet these challenges, we have undertaken a program to understand the kinetic behavior of charged particles under the combined action of electric and magnetic fields in neutral gases. A multi term theory for solving the Boltzmann equation has been developed and used to calculate transport coefficients of charged-particle swarms in neutral gases [1,2].

In the first part of this talk I will focus on non-equilibrium magnetized plasma discharges where the electric and magnetic fields can vary in space, time and orientation depending on the type of discharge and where attention must be paid to the correct treatment of temporal and spatial non-locality within the discharge. I will highlight the duality of transport coefficients arising from the explicit effects of non-conservative collisions particularly for electrons in rare gas metal-vapor mixtures, having in mind applications in lighting industry. As an example of fluid modeling of plasmas, I will discuss the recently developed high order fluid model for streamer discharges [3,4]. Starting from the cross sections for electron scattering, it will be shown how the corresponding transport data required as input in fluid model should be calculated under conditions when the local field approximation is not applicable. The temporal evolution of electron number density and electric field in the classical first order and in the high order model are compared and the differences will be explained by physical arguments.

In the second part of this talk I will discuss the detector physics processes of resistive plate chambers that are often used in many high energy physics experiments. Critical elements of modeling include the primary ionization, avalanche statists and signal development. The Monte Carlo simulation procedures that implement the described processes will be presented. Time resolution and detector efficiency are calculated and compared with experimental measurements and other theoretical calculations.

References

[1] S. Dujko, R.D. White, Z.Lj. Petrović and R.E. Robson, Phys. Rev. E **81** 046403 (2010)
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[4] A. Markosyan, S. Dujko and U. Ebert, under revision for J.Phys.D.

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Abstracts of Posters (ems)

E-06

Transport coefficients for electrons in rare-gas metal-vapor mixtures

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The progress and further improvements of light sources based on low pressure electrical gas discharges require the most accurate modeling of charged particle transport processes in rare-gas-metal-vapor mixtures [1]. In this work we investigate electron transport in mixtures of rare gases (argon and neon) and metal vapors (sodium, potassium, cesium, magnesium and mercury) under swarm conditions using a multi term theory for solving the Boltzmann equation [2]. Calculations are performed over a range of E/N values, gas temperatures and metal vapor concentrations relevant to lamp discharges. Values and general trends of mean energy, drift velocity, diffusion tensor and rate coefficients are presented in this work.

Our work has been motivated, in part, by recent suggestions that highly accurate data for transport coefficients required as input in fluid models of lamp discharges may significantly improve the existing models. Current models of such lamps require knowledge of the plasma electrical conductivity, which can be calculated from the cross sections for electron scattering in rare-gas-metal-vapor mixtures and mobility coefficients presented in this work. In addition, we discuss the duality of transport coefficients arising from the explicit effects of ionization and correct implementation of transport data in fluid models of such discharges. Special attention is paid to the determination of transport data under steady-state Townsend conditions and their relations to transport coefficients obtained under hydrodynamic conditions [3]. The effects of metastable atoms and presence of dimmers in metal vapors on the swarm parameters are also discussed. Therefore, in this work we revisit and distill the most essential aspects of the definition and calculation of transport coefficients, giving numerical results for a range of transport data in rare-gas metal-vapor mixtures required as input in fluid models of lamp discharges.

References

[1] G.G. Lister, J.E. Lawler, W.P. Lapatovich and V.A. Godyak, *Rev. Mod. Phys.* **76** 541 (2004)
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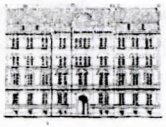

Република Србија
Универзитет у Београду
Физички факултет
Д.Бр.2012/8021
Датум: 02.02.2017. године

На основу члана 161 Закона о општем управном поступку и службене евиденције издаје се

УВЕРЕЊЕ

Мирић (Младен) Јасмина, бр. индекса 2012/8021, рођена 03.02.1987. године, Призрен, Република Србија, уписана школске 2016/2017. године, у статусу: самофинансирање; тип студија: докторске академске студије; студијски програм: Физика.

Према Статуту факултета студије трају (број година): три.
Рок за завршетак студија: у двоструком трајању студија.

Ово се уверење може употребити за регулисање војне обавезе, издавање визе, права на дечији додатак, породичне пензије, инвалидског додатка, добијања здравствене књижице, легитимације за повлашћену вожњу и стипендије.

Овлашћено лице факултета

РЕПУБЛИКА СРБИЈА

УНИВЕРЗИТЕТ У БЕОГРАДУ
ЕЛЕКТРОТЕХНИЧКИ ФАКУЛТЕТ

ДИПЛОМА

О СТЕЧЕНОМ ВИСОКОМ ОБРАЗОВАЊУ

МИРИЋ МЛАДЕН ЈАСМИНА

РОЂЕН-А 03.02.1987. ГОДИНЕ У ПРИЗРЕНУ, РЕПУБЛИКА СРБИЈА,
УПИСАН-А 2005/06.ГОДИНЕ, А ДАНА 15.9.2011. ГОДИНЕ ЗАВРШИО-ЛА ЈЕ СТУДИЈЕ НА ЕЛЕКТРОТЕХНИЧКОМ ФАКУЛТЕТУ НА ОДСЕКУ ЗА ФИЗИЧКУ ЕЛЕКТРОНИКУ-СМЕР БИОМЕДИЦИНСКИ И ЕКОЛОШКИ ИНЖЕЊЕРИНГ, СА ОПШТИМ УСПЕХОМ 8,62 (ОСАМ 62/100) У ТОКУ СТУДИЈА И ОЦЕНОМ 10 (ДЕСЕТ) НА ДИПЛОМСКОМ ИСПИТУ.

НА ОСНОВУ ТОГА ИЗДАЈЕ МУ-ЈОЈ СЕ ОВА ДИПЛОМА О СТЕЧЕНОМ ВИСОКОМ ОБРАЗОВАЊУ И СТРУЧНОМ НАЗИВУ ДИПЛОМИРАНИ ИНЖЕЊЕР ЕЛЕКТРОТЕХНИКЕ.

РЕДНИ БРОЈ ИЗ ЕВИДЕНЦИЈЕ О ИЗДАТИМ ДИПЛОМАМА 18292.
У БЕОГРАДУ, 16. 9. 2011. ГОДИНЕ.

ДЕКАН
Проф. др Миодраг Поповић

РЕКТОР
Проф. др Бранко Ковачевић

Република Србија

УУБ

Универзитет у Београду
Електротехнички факултет, Београд

Оснивач: Република Србија
Дозволу за рад број 612-00-02666/2010-04 од 10. децембра 2010. године је издало Министарство просвете и науке Републике Србије

Диплома

Јасмина, Младен, Мирић

рођена 3. фебруара 1987. године у Призрену, Република Србија, уписана школске 2011/2012. године, а дана 1. новембра 2012. године завршила је мастер академске студије, другог степена, на студијском програму Електротехника и рачунарство, обима 60 (шездесет) бодова ЕСПБ са просечном оценом 10,00 (десет и 0/100).

На основу тога издаје јој се ова диплома о стеченом високом образовању и академском називу

мастер инжењер електротехнике и рачунарства

Број: 1199300
У Београду, 28. марта 2013. године

Декан
Проф. др Бранко Ковачевић

Ректор
Проф. др Владимир Бумбаширевић

00012272

Кратак преглед научне активности кандидата

Кандидат Јасмина Мирић је ангажована на пројекту Министарства науке, просвете и технолошког развоја ИИИ41011 „Примена нискотемпературних плазми у биомедицини, заштити човекове околине и нанотехнологијама" под менторством др Саше Дујка. Кандидат се бави транспортном теоријом електрона у гасовима и моделовањем стримерских тражњења имајући на уму пре свега примене у технологији гасних диелектрика.

У првом делу свог досадашњег рада, Јасмина Мирић се посветила истраживању ударних и транспортних особина електрона у јако електронегативним гасовима. На основу постојећих података у литератури и примењујући технику ројева наелектрисаних честица, кандидат је развио комплетне сетове пресека за расејање електрона за неколико гасних диелектрика последње генерације које одликује веома низак глобални фактор за загревање атмосфере. Јасмина Мирић је учествовала у развоју нумеричких процедура за надокнађивање електрона изгубљених захватом електрона у Монте Карло симулацијама. Након развоја, детаљног тестирања и имплементације ових процедура у Монте Карло код, израчунати су транспортни коефицијенти електрона у трифлуорометил јодиду (CF_3I) и сумпор хексафлуориду (SF_6) у широком опсегу редукованих електричних поља. Највећа пажња је посвећена разумевању и анализи кинетичких феномена индукованих процесима захвата електрона. За физичко тумачење ових феномена израчунате су функције расподеле електрона и просторно разложене карактеристике роја.

У другом делу свог досадашњег рада, Јасмина Мирић се бавила проучавањем развоја електронских лавина, њиховом транзицијом у стримере и пропагацијом стримера у јако електронегативним гасовима. За ова проучавања су коришћени флуидни модели стримерских пражњења различите комплексности. У овим истраживањима акценат је стављен на повезивању микроскопских особина електрона и макроскопских особина стримерских пражњења. Дискутована је осетљивост брзине пропагације стримера и расподеле електричног поља на различите сетове пресека за расејање електрона као и на природу транспортних коефицијената који се користе као улазни подаци. Значајна пажња је посвећена разумевању ефеката рекомбинације електрона и позитивних јона као и међусобне рекомбинације различито наелектрисаних јона на развој и пропагацију стримера у јако електронегативним гасовима.

На основу нумеричких мулти терм решења Болцманове једначине и Монте Карло метода, кандидат је проучавао транспорт електрона у живиним парама на високим температурама и притисцима. Показано је да коректна репрезентација димера атома живе и супереластичних судара има кључну улогу за разумевање феномена негативне диференцијалне проводности.

Досадашњи резултати Јасмине Мирић су приказани у раду у међународном часопису изузетних вредности (М21а). Кандидат је, као коаутор, учествовао на већем броју међународних и домаћих конференција као и на неколико уводних предавања.