Publ. Astron. Obs. Belgrade No. 102 (2022), 49 - 52 *Contributed Paper*

THIRD-ORDER TRANSPORT COEFFICIENTS FOR ELECTRONS IN C_3F_8

I. SIMONOVIĆ[1], D. BOŠNJAKOVIĆ[1], Z. LJ. PETROVIĆ[2], and S. DUJKO[1]
[1] *Institute of Physics Belgrade, Pregrevica 118, 11080 Belgrade, Serbia*

[2] *Serbian Academy of Sciences and Arts, Knez Mihailova 35, 11000 Belgrade, Serbia*

Abstract. Monte Carlo simulations and multi term method for solving the Boltzmann equation are used to calculate the third-order transport coefficients for electrons in C_3F_8. The influence of elastic, inelastic and non-conservative collisions of electrons with molecules of the background gas on the individual components of the third-order transport tensor is investigated. The differences between flux and bulk values of the third-order transport coefficients are analyzed. The concurrence of the third-order transport tensor with diffusion is observed and studied.

1. INTRODUCTION

The investigation of electron transport in gases under the influence of an electric field is important for many technological applications. These applications are often modelled assuming hydrodynamic conditions in which the flux of electrons is represented in terms of drift velocity and the diffusion tensor, as higher-order transport coefficients have been systematically ignored in the traditional interpretation of swarm experiments. However, the longitudinal third-order transport coefficient has been recently measured from the arrival-time spectra of an electron swarm by Kawaguchi et al. (see Kawaguchi et al. 2021). It has been shown by Kawaguchi and coworkers that third-order and higher-order transport coefficients should be considered to obtain the longitudinal diffusion coefficient properly in the arrival-time spectra experiment at moderate and high reduced electric fields. Third-order transport coefficients are also necessary for the conversion of the hydrodynamic transport coefficients into transport data that is measured in the steady-state Townsend experiment (see Dujko et al. 2008.). If third-order transport coefficients were both calculated and measured with a sufficient precision, they would be very useful in the swarm procedure for determining the complete sets of cross sections, due to the high sensitivity of these transport coefficients to the energy dependence of cross sections for individual scattering processes (Vrhovac et al. 1999). In this work we investigate the third-order transport coefficients for electrons in C_3F_8 by employing Monte Carlo simulations and the multi term method for solving the Boltzmann equation. In section 2 we give a brief description of the methodology that is used in this work. Results and discussion are presented in section 3.

2. THEORETICAL METHODS

In our Monte Carlo simulations, we follow a swarm of electrons moving in a homogeneous background gas. The interactions between electrons are neglected due to their small number density, and the dynamics of an individual electron is determined by the electric field and by collisions with the molecules of the background gas. In these simulations random numbers are extensively employed in order to determine the time and the type of the next collision as well as postcollisional velocity of an electron. Transport coefficients are calculated from polynomials of the components of the position and velocity vectors of individual electrons, which are averaged over the entire swarm. The details of our Monte Carlo code are given in previous papers (see Dujko et al. 2010.). The bulk values of the third-order transport coefficients are determined from

$$\mathbf{Q}^{(b)} = \frac{1}{3!}\frac{\mathrm{d}}{\mathrm{d}t}\langle \mathbf{r}^{\star}\mathbf{r}^{\star}\mathbf{r}^{\star}\rangle, \tag{1}$$

while the flux third-order transport coefficients are calculated as:

$$\mathbf{Q}^{(f)} = \frac{1}{3!}\left\langle \frac{\mathrm{d}}{\mathrm{d}t}\left(\mathbf{r}^{\star}\mathbf{r}^{\star}\mathbf{r}^{\star}\right)\right\rangle, \tag{2}$$

where $\mathbf{r}^{\star} = \mathbf{r} - \langle \mathbf{r}\rangle$, and the brackets $\langle\rangle$ represent ensamble averages. As these expressions have pronounced statistical fluctuations, a large number of electrons (at least 10^7) are followed in our Monte Carlo simulations in order to determine the third-order transport coefficients.

In the second method that is used in this work we employ numerical solutions of the Boltzmann equation. The Boltzmann equation represents the equation of continuity in the phase space, and it can be written as:

$$\frac{\partial f(\mathbf{r},\mathbf{c},t)}{\partial t} + \mathbf{c}\cdot\frac{\partial f(\mathbf{r},\mathbf{c},t)}{\partial \mathbf{r}} + \frac{q}{m}\mathbf{E}\cdot\frac{\partial f(\mathbf{r},\mathbf{c},t)}{\partial \mathbf{c}} = -J(f,f_0), \tag{3}$$

where q and m are electron charge and electron mass respectively, $\mathbf{E}$ is electric field and J is collision operator. In the multi term method the phase space distribution function is expanded in terms of the spherical harmonics and Sonine polynomials in angular and radial parts of the velocity space, respectively. Under hydrodynamic conditions, the dependence of the phase space distribution function on the coordinates from the configuration space is expressed in terms of the density gradient series expansion. Then the Boltzmann equation is decomposed into a hierarchy of equations in terms of the coefficients in this expansion (the moments of the distribution function). Transport coefficients are then expressed in terms of these moments and this hierarchy of equations is truncated when the convergence of the transport coefficients is reached. The details of the multi term method, which is employed in this work, are given in previous papers (see Dujko et al. 2010.). Expressions for those components of the flux third-order transport tensor, which are independent in the electric field only configuration, are given by the following equations:

$$Q^{(f)}_{xxz} = \frac{1}{\sqrt{2}\alpha}\left[\mathrm{Im}(F(011|221;\alpha)) - \mathrm{Im}(F(01-1|221;\alpha))\right], \tag{4}$$

$$Q^{(f)}_{zxx} = -\frac{1}{\alpha}\left[\frac{1}{\sqrt{3}}\mathrm{Im}(F(010|200;\alpha)) + \frac{1}{\sqrt{6}}\mathrm{Im}(F(010|220;\alpha))\right] + \frac{1}{\alpha}\mathrm{Im}\left[F(010|222;\alpha)\right], \quad (5)$$

$$Q^{(f)}_{zzz} = \frac{1}{\alpha}\left[\sqrt{\frac{2}{3}}\mathrm{Im}(F(010|220;\alpha)) - \frac{1}{\sqrt{3}}\mathrm{Im}(F(010|200;\alpha))\right], \quad (6)$$

where Im denotes imaginary parts of the moments of the phase space distribution function, and the z-axis is directed along the electric field.

3. RESULTS AND DISCUSSIONS

In this section we show the calculated values of the third-order transport coefficients, which are obtained by employing the methods described in the previous section. The calculation of the third-order transport coefficients by employing these two methods is described more thoroughly in our previous paper (see Simonović et al. 2022.). The cross section set for electron scattering on C_3F_8 molecules, that is used in these calculations, has been developed by Biagi (see Biagi).

In figure 1.a we show all three components of the skewness tensor for electrons in C_3F_8 that are independent in the electric field only configuration. These results are obtained by using the multi term method for solving the Boltzmann equation. The $n_0^2 Q_{zzz}$ component has two local maximums and one local minimum, $n_0^2 Q_{xxz}$ component has three local maximums and two local minimums, while the $n_0^2 Q_{zxx}$ component has two local maximums and two local minimums.

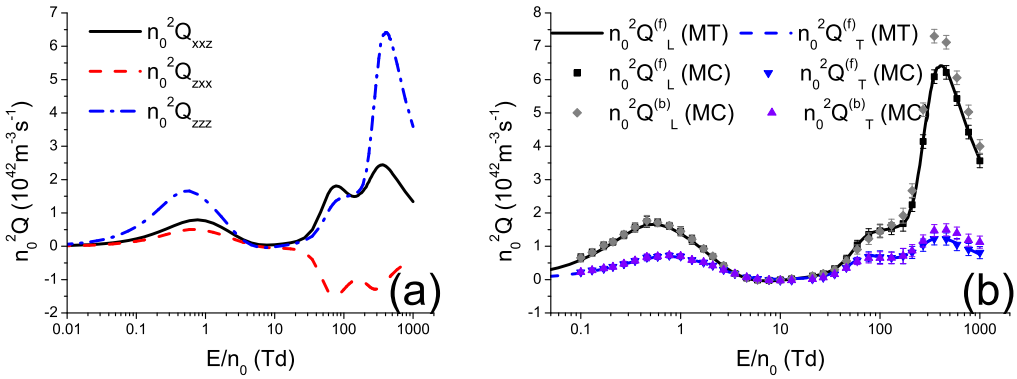

Figure 1: Independent components of the third-order transport tensor (a) and comparison of bulk and flux values of $n_0^2 Q_L$ and $n_0^2 Q_T$ (b) for electrons in C_3F_8.

In figure 1.b we show the comparison between bulk and flux values of $n_0^2 Q_L$ and $n_0^2 Q_T$. Bulk values are obtained by using Monte Carlo simulations, while flux values are determined by employing Monte Carlo simulations and the multi term method for solving the Boltzmann equation. Flux values that are obtained by using these two independent methods are generally in a good agreement, which verifies the validity of these two methods. At high electric fields bulk values are higher than the corresponding flux values, due to explicit effects of electron impact ionization.

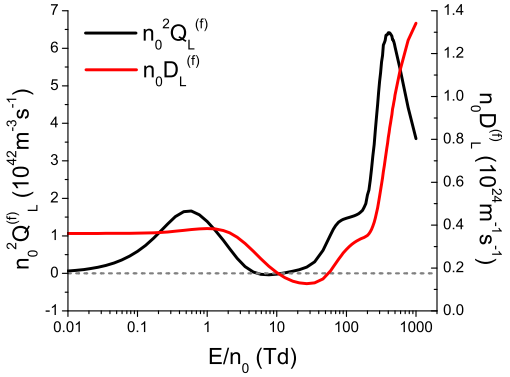

Figure 2: Concurrence between $n_0^2 Q_L^{(f)}$ and $n_0 D_L^{(f)}$ for electrons in C_3F_8.

In figure 2 we show the concurrence between $n_0^2 Q_L^{(f)}$ and $n_0 D_L^{(f)}$. This concurrence implies that $n_0^2 Q_L^{(f)}$ is being reduced with increasing E/n_0 when $n_0 D_L^{(f)}$ is being reduced, or when it increases as a concave function of E/n_0 (see Simonović et al. 2022.). The observed concurrence can be attributed to the high sensitivity of the third-order transport coefficients to the elementary scattering processes, which quench diffusive motion. It can be seen in figure 2 that $n_0^2 Q_L^{(f)}$ has a local maximum and it starts to decrease at about 0.59 Td where $n_0 D_L^{(f)}$ becomes a concave function of E/n_0. It can also be seen that $n_0^2 Q_L^{(f)}$ has a local minimum at about 8 Td, and it starts increasing at higher fields, although $n_0 D_L^{(f)}$ continues to decrease up to about 27 Td. However, $n_0^2 Q_L^{(f)}$ has negative values between approximately 5 Td, and 11 Td, and the concurrence with diffusion is violated in the vicinity of the field region where $n_0^2 Q_L^{(f)}$ is negative, as in the case of CF_4 (see Simonović et al. 2022.). Between approximately 70 Td and 170 Td, the rise of both functions slows down, while this rise becomes rapid again at higher fields. In the field region between approximately 400 Td and 1000 Td $n_0 D_L^{(f)}$ becomes a concave function of E/n_0, while $n_0^2 Q_L^{(f)}$ is being reduced with increasing field.

Acknowledgment

This research was supported by the Institute of Physics Belgrade, and the Science Fund of the Republic of Serbia [Grant No. 7749560, EGWIn].

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