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Supercomputer simulation of electron avalanches in gases with calculation of diffusive characteristics

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1 Introduction

We consider the problem of electron transfer in a gas under the action of a strong external electric field. Electrons started at the initial (zero) time moment from the cathode move with an acceleration to the anode. For the sake of simplicity, we assume that the anode and cathode are plane-parallel. Electrons move, collide with gas molecules, and then are absorbed, or diffused elastically or non-elastically, or ionize the gas "beating out" secondary electrons. Thus, the number of charged particles grows exponentially, that forms ionized gas particles and an electron avalanche (or electron cloud). The basic transport characteristics of an avalanche are diffusion coefficients (longitudinal D_L and transversal D_T ones), the drift velocity of the cloud, mobility of electrons, frequency of ionization, mean kinetic energy, primary ionization coefficient (see, e.g., [1]). This work is focused on calculations of D_L and D_T by the Monte Carlo method.

2 Formulation of the problem

The mathematical model of transfer of charger particles in an external electric field is described by the following transfer equation (see, e.g., [9]):

$$\frac{\partial f}{\partial t} + \mathbf{v}\frac{\partial f}{\partial \mathbf{r}} + \frac{q\mathbf{E}}{m}\frac{\partial f}{\partial \mathbf{v}} = \nu_c \int\limits_{\Omega'} [f(\mathbf{r}, \mathbf{v}', t) - f(\mathbf{r}, \mathbf{v}, t)] w(\omega, \omega') d\omega'. \qquad (1)$$

Here $f(\mathbf{r}, \mathbf{v}, t)$ is the electron distribution density, $\mathbf{r} = (x, y, z)$, t is the time, $\mathbf{v}$ is the velocity vector, q is the charge of a particle, $\mathbf{E}$ is the electric field vector, m is the mass of a particle, ν_c is the frequency of collision of articles with elements of the medium, $\omega = \mathbf{v}/V$, $\omega' = \mathbf{v}'/V'$ are the motion direction vectors before collision and after it, V is the absolute value of the velocity.

Special algorithms of statistical modelling are constructed to solve this equation by Monte Carlo method. Since (1) admits reduction to an integral equation, it is possible to construct motion trajectories of particles by the usual technique, which corresponds to a probabilistic physical model of electron transfer process (see, e.g., [1]).

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It is possible to calculate diffusion coefficients in several ways. One of them was proposed within the framework of diffusion approximation, i.e., for Gaussian approximation of the density. However, it can be also used for more accurate estimates of the required functionals. In this method the diffusion coefficients are obtained using the "radii" of transversal and longitudinal diffusion $R_T = \sqrt{4D_T t}$ and $R_L = \sqrt{4D_L t}$, respectively. Let the electrons begin their motion at the point with the coordinates $(x, y, z) = (0, 0, 0)$ and the electric field intensity equal $\mathbf{E} = (0, 0, -E_z)$. Thus, the electron cloud moves along the axis OZ. For the distribution density of particles $\rho(x, y, z, t)$ we obtain

$$\rho(0, y, z, t)/\rho(R_T, y, z, t) = e^{R_T^2/(4D_T t)} = e^1,$$

$$\rho(x, y, z_{max}, t)/\rho(x, y, z_{max} + R_L, t) = e^{R_L^2/(4D_L t)} = e^1.$$

Therefore, to calculate the diffusion radii we have to construct the graph of the distribution density of particles, determine the point of its maximal value ("top" point) and the point where the value of the graph is e times less than at the top point. It is clear that the sufficiently accurate calculation of the diffusion coefficients requires construction of sufficiently accurate global estimators of the density. A histogram and a polygon of frequencies with especially chosen steps were used previously for that purpose (see [1, 2]). In this work we construct more precise estimators for the diffusion radius based on the smoothed estimators of particles distribution density, namely, kernel estimators of ParzenRosenblatt [3] using a grouped sample and randomized projection method utilizing Laguerre and Hermite polynomials.

The calculations were performed by ELSHOW package in the Siberian Supercomputer Center of SB RAS with the use of PARMONC package for parallel computations [4].

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