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# Self-consistent Monte Carlo simulation of particle motion and photon transport in the Argon positive column

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**Abstract.** A highly accurate self-consistent Monte Carlo method including charged and neutral particle motion and resonance photon transport is developed and applied to the simulation of the positive column of Argon discharge. The distribution of power loss across the tube is investigated. It is shown that negative slope of the current–voltage gradient curve can not be explained by only one factor. Diffusion of metastable atoms to the tube wall in the case of low current (0.2–3 mA) is responsible for the most part of negative slope. For the high currents the variation of radiation power loss makes a main contribution to the amplitude of the negative slope.

## 1. Introduction

The positive column (PC) of gas discharge has been experimentally studied for a long time, but there is still a lack of simulation techniques able to reproduce discharge properties in much detail.

As is well established, the electron component of a discharge generally reaches a state far from the thermodynamic equilibrium. Hence, the temporal and spatial distributions of anisothermic plasmas can be described only on an appropriate microphysical basis. The most suitable approach uses the technique of particle-in-cell (PIC) simulation coupled with Monte Carlo (MC) event selection (for short, MC notation is used instead of PIC-MC; see the details of the method in [1, 2]).

In the MC algorithm the particles are considered to move classically during a period of free flight under the influence of an electric field determined by electron and ion density according to Poisson's law. The free flight is interrupted by scattering by neutral atoms, ionization, excitation, wall loss and other kinds of collisions which must be considered in the model of discharge. The free flight length and outcome of these events are selected randomly from known probability distributions.

In addition to the standard MC technique we have developed a new simple MC treatment of resonance photon transport. The new MC algorithm for photons, coupled with the tracing of electron and ion motions, results in self-consistent MC simulation of discharge. Except for an outline of the new MC method for radiative transport, we omit the detailed discussion of input data (cross sections, etc.), PIC-MC particulars and most of the simulation results due to space limitations. A detailed description of the method and simulation data can be found in [3].

## 2. Particle transport processes

In the present model the first 14 excited Ar levels are taken into consideration. The 15th level of Argon $Ar_{15}(3d_a)$ is a combined level that represents a great number of the higher excited atomic levels as one state. The electron excitation and ionization cross sections are taken from [4, 5]. The cross section of the super-elastic collisions is calculated according to the principle of detailed balance [6].

In the MC model we consider elastic electron–Ar scattering by using the published momentum transfer cross section [7]. After elastic collision, an electron is redistributed isotropically in the center-of-mass (CM) system. All ions and electrons reaching the tube wall recombine and produce the neutral atoms that are uniformally redistributed by program uniformly within tube domain. To describe electron–electron collisions by MC simulation we are the using the classical Coulomb cross section. The electron–ion and ion–ion elastic collision processes are also included in the model in the same manner as for electron–electron collision. However, according to our simulation these processes do not play any significant role in the PC.

Ion transport in the ion-parent-atom case is mostly guided by resonant charge transfer because its cross section is large at low collision energies. We use simple fitted functions for the charge transfer and polarization scattering cross section [6].

The simple treatment of diffusion based on an equation of continuity is included in the model. The flux of atoms is estimated on the basis of Fick's law. The charged particle is considered to move classically during the period between collisions (free flight) under the influence of a self-consistent electric field within the discharge tube. This field is determined by electron and ion density according to Gauss's law.

## 3. Resonance radiative transport

Due to the high absorption of the resonance photons by atoms in the ground state the correct treatment of radiative transfer in the discharge condition is crucial for the model. Our MC simulation of traveling photons is based on Biberman–Holstein theory [8] of resonance radiative transport.

Let us denote by $\rho(r) = k\exp(-kr)$ the probability density of a photon captured within $[r, r+dr]$ and without absorption along distance $[0, r]$. Then the probability of the absorption anywhere within $[0, R]$ is $\int_0^R \rho(r)\,dr = 1 - \exp(-kR)$ and the probability of the traversing a distance $R$ is $T(R) = 1 - \int_0^R \rho(r)\,dr = \exp(-kR)$. Due to line broadening the absorption coefficient $k$ depends on a photon frequency $\omega$.

In a general case the emission/absorption line shape is determined by Doppler broadening, as well as natural and pressure broadening. The combination of these effects may be given by the Voigt profile

$$h(a,x) = \frac{a}{\pi}\int_{-\infty}^{\infty} \frac{\exp(-y^2)\,dy}{a^2 + (x-y)^2},$$

where $x$ is dimensionless frequency and $a$ is the Voigt parameter. The general form of transmission probability density can be rewritten for this profile as follows

$$\rho(k_0 r) = \frac{k_0}{\sqrt{\pi}}\int h^2(a,x)\exp\left[(-k_0 h(a,x) r\right]dx, \tag{3.1}$$

where $k_0$ is an absorption coefficient at the maximum of the line profile.

To generate a random number according to the probability density $\rho(k_0 r)$ given by (3.1) we develop a new simple random generator

$$k_0 r = \left(X^{-2} - 1\right)/2, \quad \text{with comparison function} : f(k_0 r) = 2/(1 + 2k_0 r)^{3/2} \quad (3.2)$$

In the first step the program generates a trial random number $k_0 r$ according to (3.2) by using a random number $X$ uniformly distributed within $[0, 1]$. In the second step another random number $Y \in [0, 1]$ is picked. If $Y > \rho(k_0 r)/f(k_0 r)$, then the program rejects the trial number $k_0 r$ and returns to the first step. Otherwise the program accepts the $k_0 r$. The efficiency of this generator is equal to 50% because of $\int f(k_0 r) d(k_0 r) = 2$. The testing of the random generator (3.2) indicates that the simulated probability density is in excellent agreement with the theoretical function from (3.1). The transmission probability density $\rho(k_0 r)$ is evaluated and stored in a file which is later used by the MC program.

It is significant to note that the resonance photon reflection from the tube surface cannot be neglected. The specular reflection of a tube material is described by the generalized Fresnel reflection coefficients. The MC program calculates the path including (one or many) reflections of resonance photon beam within a tube and converts it to resonance excited atom states at the final location (see the details in [3]).

## 4. Simulation results

Electrons acquire kinetic energy from the axial electric field $E_z$ in a tube, from superelastic collisions, and from excited atom–atom ionization and lose it in ionization, elastic electron–atom(ion), exciting electron–atom, and electron–tube wall collisions. Ions gain kinetic energy mostly from the radial electric field $E_\mathrm{r}$ and lose it in the ion–atom and ion–wall collisions. Excited atoms in their turn gain/lose energy by the electron hits and radiative transitions, and lose energy by diffusion to the tube wall. Our MC program provides detailed information on all of these processes included in the discharge model. Simulation data show that the MC program can reproduce with a good accuracy the experimental voltage–pressure and voltage–current curves in the PC of Argon [9, 10] (see, for comparison, Fig. 1).

The input electric power must be qual to the total wasted power at a steady PC

$$W = IE_z = \sum W_n \quad (4.1)$$

The program calculates independently the input electric power $W = IE_z$ and the dissipated powers $W_n$ for each energetic $n$-channel such as light emission, electron–atom and ion–atom elastic collisions, ionization, diffusion of excited atoms to the tube wall, and electron–wall and ion–wall losses. Simulation shows that the power balance maintains with a good precision. To reveal the influence of dissipating $n$-channels on the axial electric field we may rewrite (4.1) as

$$E_z = \sum W_n/I = \sum E_n \quad (4.2)$$

where $E_n$ is a partial axial field which corresponds to $n$-channels of the total power dissipation. By using the partial electric field $E_n$ one may estimate the contribution of each $n$-channel to the total energy loss in a steady PC and, moreover, determine the real atomic reasons behind the variation of measured axial electric field $E_z$.

The negative slope $\Delta E_z$ in $E$–$I$ curve in Fig. 1(a) can be decomposed into partial components $\Delta E_n$ of total electric field $E_z$ according to the equality

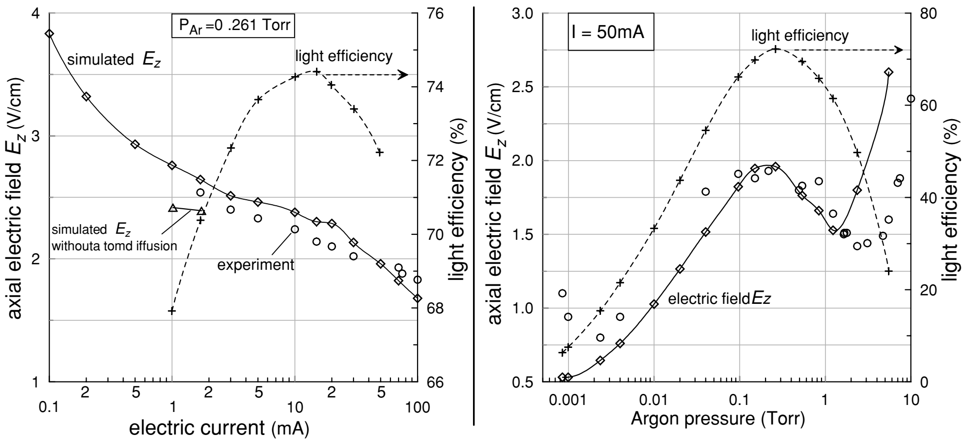


**Figure 1.** Voltage–current (a) and voltage–pressure (b) characteristics of the PC in Argon (tube diameter 1.95 cm), and the efficiency of total light emission to the total power dissipated in the PC. Triangles corresponds to simulation without diffusion of excited atoms to the tube wall. Circles denote the experimental data by Gross [9].

**Table 1.** $\Delta E_n/\Delta E_z$ (%) contributions of the partial power dissipations in $E$–$I$ slope.

| Current (mA) | Diffusion | ion–Ar collision | Radiation | Ionization | Electron–wall | Ion–wall |
|---|---|---|---|---|---|---|
| 0.02 − .05 | 13.5 | 27.8 | 30.0 | 22.5 | 5.7 | 0.8 |
| 0.1 − 0.2 | 29.2 | 20.4 | 31.9 | 16.2 | 3.1 | 0.1 |
| 0.5 − 1.0 | 54.2 | 18.4 | 13.7 | 14.5 | 2.4 | −1.8 |
| 3.0 − 10 | 31.7 | 20.5 | 40.4 | 13.3 | 1.6 | −6.5 |
| 30 − 100 | 0.8 | 7.0 | 89.3 | 3.7 | 0.1 | −1.9 |

$1 = \sum_n \Delta E_n/\Delta E_z$ from (4.2). As shown in Table 1, the most considerable (not for $E_z$ but for the derivative $dE_z/dI$) power loss channel is the diffusion of metastable atoms to the tube wall in the case of low current (0.2–3 mA). For the high currents the variation of radiation power loss makes the main contribution to the amplitude of negative slope.

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