

PIC/Monte Carlo Simulation of Dielectric Barrier Discharge in Argon

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Abstract

The present work deals with the study of an atmospheric pressure Argon plasma in a parallel-plate dielectric barrier discharge (DBD) by a one-dimensional particle-in-cell/Monte Carlo code, supposing that the reactor gap is much smaller than the plate area of electrodes. Electron-neutral collisions, both elastic and inelastic, have been considered, including superelastic collisions and electron impact ionizations. The kinetic model has been coupled self-consistently with a proper electric circuit model.

1. Introduction

Interest in dielectric barrier discharges (DBD) for plasma actuators has seen an important growth in the last years. A barrier discharge occurs when an alternating high voltage is applied to conductive electrodes, at least one of them covered with a dielectric layer, allowing only the passage of the displacement current, acting as a current limiter and preventing the formation of an arc discharge. The electrical energy of a DBD plasma is mainly transferred to electrons, while the neutral gas remains closest to the ambient temperature. DBD has many applications such as sterilization and bacteria inactivation, surface treatment and activation, and excimer formation [1]. One-dimensional models for the dielectric barrier discharge dynamics are based on the numerical solution of the electron and ion continuity and momentum transfer equations coupled to Poisson equation, developed to optimize the design of a DBD reactor over a wide range of discharge conditions [2]. Typically an optimal discharge gap or applied voltage can be found by employing these models in order to optimize the average power consumption. However, fluid simulations cannot achieve the detailed kinetic behavior which, in contrast can be obtained by using Particle-In-Cell (PIC) simulations [3]. In the next Section a detailed description of the physical and numerical model developed is carried out and some results have been reported in the

last section.

2. Physical and numerical model

The parallel-plate electrode–dielectric configuration used in the simulation is sketched in Fig. 1, where dielectric plates are bounded by planar metal electrodes and self-consistently coupled with an external circuit. A 1D coupled model is built to describe the Argon discharge under the assumption that the discharge characteristic is uniform in the transversal direction.

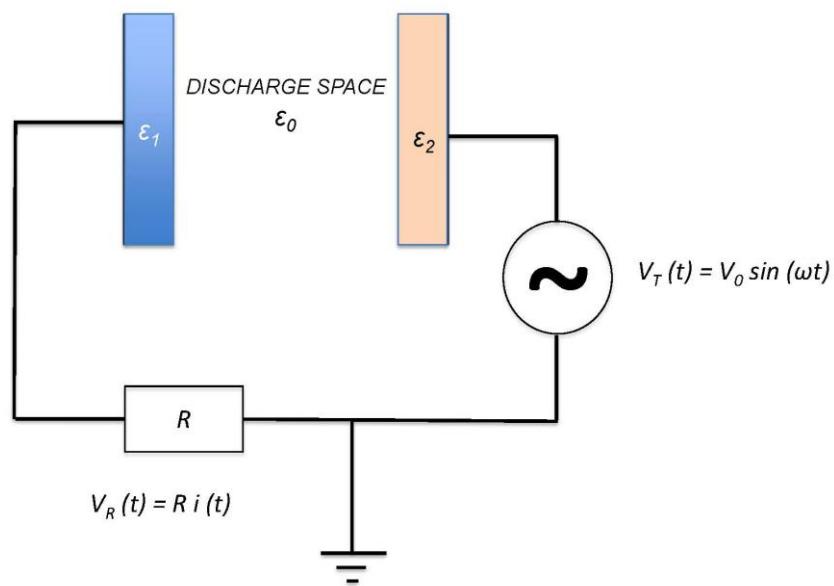


Fig.1 Sketch of the electrode configuration discharge and of the external circuit.

In the Poisson solver, the surface charge on all dielectrics are included by self consistently accounting for the deposited surface charges, as well as the dielectric coefficients. Moreover, perfect dielectrics have been considered with null conductivity and no charge leaking. For the Poisson equation, the potential of the grounded electrode is $V_R(t)$, and a sinusoidal voltage $V_T(t)$ is applied on the high-voltage electrode as shown in Fig. 1. The surface charge density deposited on the dielectric barriers is calculated following the dynamics of the computational particles and, according to Gauss' law, the boundary condition of interfaces between the dielectric and discharge space is evaluated. Finally, neglecting the influence of space charge in the dielectric barrier, electric field is calculated by means of the Laplace's equation.

Four kinds of particles, electrons (e), ion (Ar^+), ground, Ar, and excited states Ar^* , are considered and four reactions (R1-R4) are included in the present model and listed in Table I, i.e., elastic, superelastic [5], electron excitation and ionizations.

Table 1. List of reactions of electron with Argon (excited argon atoms Ar^* : all of the excited atoms in 4 s level, argon atom Ar, singly ionized argon atom Ar^+).

| Reaction | Formula | Type | ΔE (eV) |
|----------|---|--------------|-----------------|
| R1 | $\text{e} + \text{Ar} \rightarrow \text{e} + \text{Ar}$ | elastic | |
| R2 | $\text{e} + \text{Ar} \rightarrow \text{e} + \text{Ar}^*$ | excitation | 11.5 |
| R3 | $\text{e} + \text{Ar}^* \rightarrow \text{e} + \text{Ar}$ | superelastic | -11.5 |
| R4 | $\text{e} + \text{Ar} \rightarrow \text{e} + \text{Ar}^+$ | ionization | 15.8 |

Collisions have been accounted for by using the Monte Carlo collision method (MCC) [5] during the discharge transient. Neutrals and electrons are initially at rest and distributed uniformly inside the discharge region by using pseudorandom numbers. Simulations have been repeated averaged in order to obtain the ensamble average [6].

3. Results

Simulations have been performed under different conditions, varying dielectric constant and geometry of the system (gap length, thicknesses and characteristics of the dielectric, amplitude and frequency of the applied voltage).

As an example, Fig. 2 shows the time evolution of the electrical characteristics of the discharge across the gap. The change in current depicts breakdown of the gap, started when the gas voltage reaches values above the breakdown voltage.

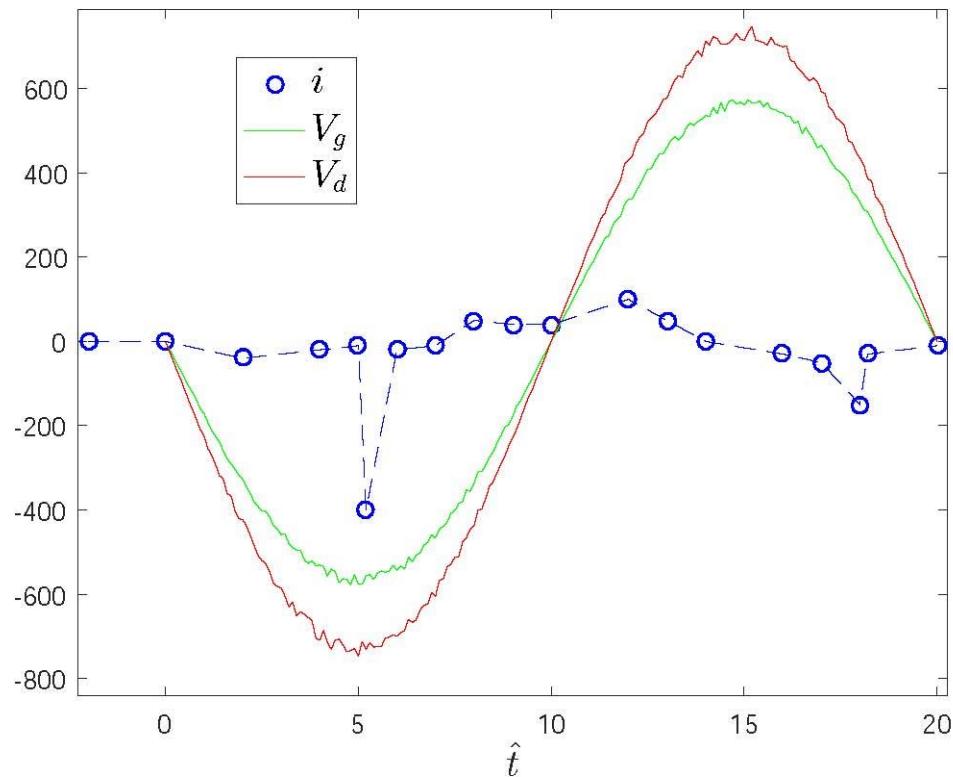


Fig.1 Time evolution of the current (blue dashed line with circles), gas voltage (green full line) and discharge voltage (red full line). In the numerical code all the quantities have been properly normalized.

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