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Effect of plasma chemistry on the simulation of helium atmospheric-pressure plasmas

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ABSTRACT

The effect on the selection of different plasma chemistries for simulating a typical dielectric barrier discharge (DBD) driven by quasi-pulsed power source (20 kHz) is investigated. The numerical simulation was performed by using the one-dimensional self-consistent fluid modeling solver. Our simulation result indicates that the computed temporal current density can be significantly improved by using a complex version of plasma chemistry module rather than the simple one and demonstrates an excellent agreement with the experimental data. The result suggests the metastable, excited and ionic helium related reaction channels, which are important in simulating a DBD, should be taken into account. Furthermore, it also reveals that the power absorption of ions is considerably higher than that of the electron.

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1. Introduction

Atmospheric-pressure plasmas (APP) have attracted tremendous attention in the past two decades. Without using vacuum equipment, APP helps to keep costs dramatically down during materials processing and offers the possibility of in-line processing in industry. In addition, APP has numerous applications in modern science and technology, including surface cleaning, surface modification, thin film deposition, etching, biological decontamination, ozone generation, pollution control, flat plasma display panels, and gas lasers, to name a few [1]. Studying these APPs thus becomes a hot research topic, and helium dielectric barrier discharge (DBD) especially represents one of the most useful and important ones.

Besides experimental approaches, the numerical simulator based on fluid modeling has been demonstrated to be a very useful tool for understanding both of plasma physical and chemical characteristics of helium discharges [2]. Indeed, an appropriate selection of the plasma chemistry, as well as the numerical accuracy can be achieved by a solver are key factors in success of the helium DBD simulation. However, it seems that there was no previous research addressing the issue on the effect of selected different plasma chemistry modules in the helium DBD simulations driven by complicated applied voltage waveform and presenting the direct validations with experimental data.

2. Fluid modeling equation solver

In this study, a parallel fully implicit one-dimensional self-consistent fluid modeling solver is employed to simulate the helium plasmas DBD (quasi-pulsed 20 kHz). In the framework of fluid modeling [3], the governing equations we consider include the continuity equations with drift-diffusion approximation for both of electron and ions, the continuity equation for neutral species, the energy density equation for electron and Poisson's equation for electrostatic distribution. In our model, the flow convection effects are neglected and the drift and diffusion coefficients and the rate constants related to electrons are the function of the electron temperature. These functional relations obtained by a publicly available Boltzmann equation solver, BOLSIG+ [4], are prepared as a lookup table during the preprocessing stage in the computer code. Due to the page limit, we skip the description of our fluid modeling solver and refer interested readers to [5] for details. The solver is used for simulating the helium discharge using both complicated [6] (see Fig. 1) and simple [7] plasma chemistry modules. Note that the complicated plasma chemistry module has more metastable, excited and ionic helium related reaction channels compared to simple one (not shown here). As shown in the next section, these channels are important in faithfully simulating a helium DBD.

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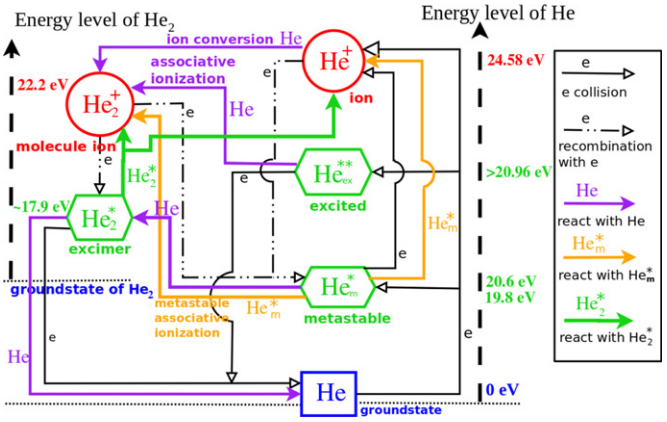

Fig. 1. Complex helium plasma chemistry applied in the present DBD simulation.

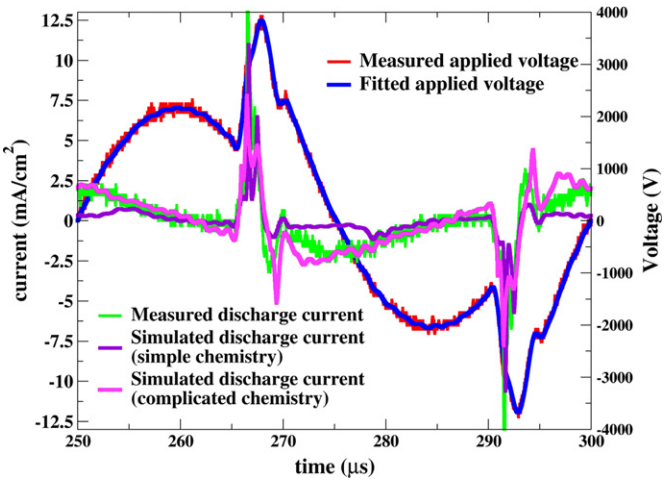

Fig. 2. A comparison of the simulated results and the measured data for the discharged currents.

3. Results and discussion

Fig. 2 shows a comparison of simulated results with experimental discharged currents of a DBD driven by a quasi-pulsed power source with measured permittivity of $11.63\varepsilon_0$. Note the currents are calculated by a product of the current density and the area (25 cm^2) in the experiments. The maximum current density is roughly 10 mA/cm^2, which is a typical Townsend-like discharge. This can be confirmed by the detailed snapshots of the number density distribution of various charged particles (not shown here due to page limit), which show that the electron number density is in general much less than the ion number density for all times. This also influences the magnitude of electrical power absorbed by the charged particles, which can be seen in Fig. 3 and will be explained later.

We also observe from Fig. 2 that the computed temporal currents by using a complex plasma chemistry module agree excellently with the measurements, while those obtained by using simple plasma chemistry module fail to reproduce the measurements in some periods of a cycle. Such discrepancy includes the over-prediction of major discharge current peaks and the under-prediction between major current peaks. This implies that the ionic and excited/metastable helium related reactions need to be taken into account for simulating helium DBD. The discrepancy can be attributed to the higher power absorption by these ionic particles by the relatively low-frequency power source compared to radio frequency, which is shown next.

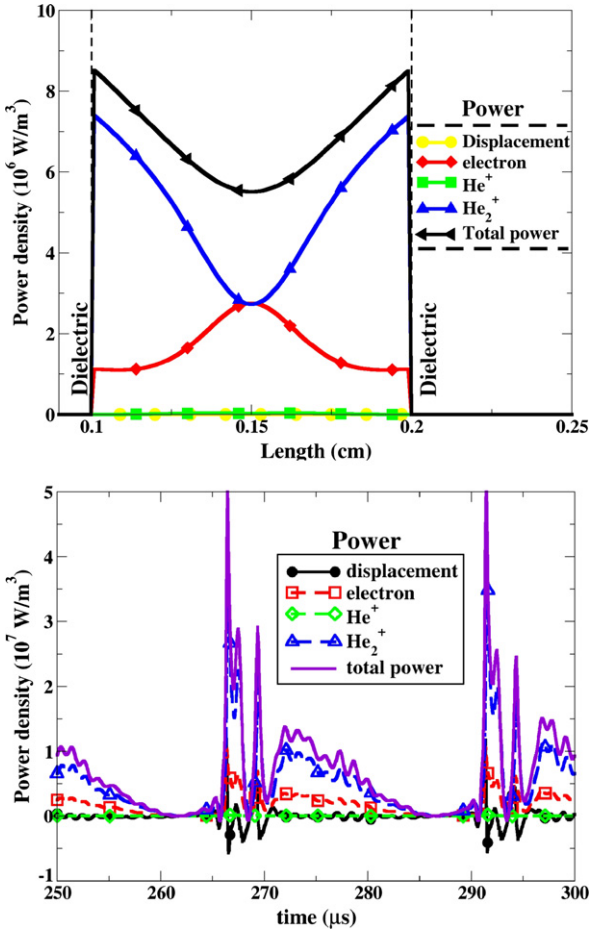

Fig. 3. Time-averaged spatial (top) and spatial-average temporal (bottom) power absorption for different mechanisms.

Fig. 3 shows the time-averaged spatial and spatial-averaged temporal power absorption for various mechanisms and the results indicate that most of the power is absorbed by the molecular helium ions, rather than by the electrons, which is very different as compared to the case of RF (radio frequency) helium discharge. Also the power absorption by the atomic helium ion is much less than that by the molecular one and the electrons due to much lower concentration in the discharge, because of Townsend-like discharge. One explanation is that the slow oscillating voltage waveform provides enough time for the molecular helium to accelerate in the electric field leading to much higher power absorption through ohmic heating.

4. Conclusion

The effect on the selection of the plasma chemistry for simulating helium DBD is presented in this study. Our numerical results suggested that the inclusion of more helium related ion, excited and metastable related reaction channels is important in reproducing measured discharged current. Attributed to the existence of fewer electrons (Townsend-like) and the application of slower oscillating electric field for a DBD, molecular helium ions absorb much more energy through ohmic heating than electrons. In general, by adopting the complex plasma chemistry module, our one-dimensional fluid modeling solver can faithfully reproduce the measured currents of helium DBD quantitatively, which has not been found in the literature, to the best knowledge of the authors.

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