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Simulation of high frequency short pulse excitation of co-axial xenon excimer source for generation of 172 nm radiation

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Dedicated to Prof B N Basu

In this work, simulation study of dielectric barrier discharge-based xenon excimer source of co-axial geometry radiating at 172 nm is carried out. The discharge is ignited in the 4 mm gas gap between the metallic electrode and the dielectric covered grounded electrode. The spatio-temporal characteristics of the source has been investigated for the pulsed voltage of amplitude 5 kV repeated with the frequency of 25 kHz. The investigation has been done for two cases of gas pressure, 100 mbar and 150 mbar, in order to achieve higher concentration of Xe_2 excimer. It has been found that the concentration of the xenon excimer is higher for the gas pressure of 150 mbar which is near to the cathode. © Anita Publications. All rights reserved.

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1 Introduction

Dielectric barrier discharges are widely used in the generation of ultraviolet radiation and established itself as an alternative option of conventional mercury-based discharge source for UV generation [1]. The characteristics of the DBD are well suited for the operation of excimer sources for the generation of VUV/UV radiation. These sources emit various spectral output characteristics depending on the gas that is participating in the discharge mechanism [2-4]. The generated radiation of different wavelengths is useful for different applications such as bacterial inactivation, surface modification, Radiotherapy, virus disinfection, water purification etc [1,5-7]. Noble gases or a mixture of noble gas and halogen are used in the excimer sources. These types of mercury free excimer sources are environment friendly and are gaining continued importance in present day applications. Excimer sources filled with xenon gas at higher pressure for the generation of 172 nm VUV radiation have various applications in material processing. These sources are typically having a planar or cylindrical geometry with a single or double dielectric barrier powered by AC voltage in the kHz range. Over the last two decades, a good extent of studies are devoted in extending the investigation of short pulsed and RF-operated dielectric barrier discharges [8-10]. The electrical to the optical conversion efficiency of the sinusoidal voltage excited Xe DBD excilamp is in the range of 10-20% due to the occurrence of filamentary micro discharges distributed across the dielectric surface [10]. Some works reported that the electrical-to-optical conversion efficiency of the DBD-based Xe excilamp got remarkably increased to greater than 60% by applying the pulsed voltage [11]. Experiments and theoretical investigations have been carried out to understand the dynamic processes of the plasma in the DBD-based Xe lamp for achieving higher conversion efficiency adopting pulsed voltage operation [12,13]. Different simulation models have also been

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developed to investigate the effect of applied voltage waveforms of different shapes [8,12,14]. Operating and geometrical parameter both significantly affects the efficiency of excilamp. Further investigations are required to be pursued in order to determine the simultaneous effects of these parameters towards controlling the reaction mechanism for efficient operation.

In this paper, simulation study of single barrier co-axial Xenon excimer source excited by pulsed dielectric barrier discharge has been carried out. The simulation has been performed using the 1-D fluid model in the COMSOL Multiphysics software [15] at two conditions of gas pressure i.e 100 and 150 mbar respectively. The model describes the spatio-temporal characteristics of the excimer source excited by the pulsed voltage of magnitude 5 kV repeated with the frequency of 25 kHz.

2 Model Description

The model is one-dimensional in the radial direction which describes the evolution of electrons, atomic ions and other neutral species radially in the co-axial lamp at different instants of time assuming that the discharge is homogeneous in the other direction. The spatio-temporal behaviour of the xenon plasma at medium pressure in the co-axial geometry has been studied here by using a set of equations described in the simulation model [12]. The simulated geometrical structure uses the single dielectric barrier for the controlled discharge on the application of a pulsed voltage of a sub-microsecond regime. The processes or plasma chemistry of the xenon used in the model is describe below:

Elastic Collision	$e + Xe \Longrightarrow e + Xe$
Electron impact excitation	$e + Xe \Longrightarrow e + Xe_1$
Electron impact de-excitation	$e + Xe_1 \Longrightarrow e + Xe$
Electron impact ionization	$e + Xe \Longrightarrow 2e + Xe^+$
Stepwise ionization	$e + Xe_1 \Longrightarrow 2e + Xe^+$
Dimer formation	$2Xe + Xe_1 \Longrightarrow Xe_2 + Xe$
Penning Ionization	$Xe_2 + Xe_2 \Longrightarrow e + 2Xe + Xe_2^+$
Penning Ionization	$2Xe + Xe^+ \Longrightarrow Xe + Xe_2^+$
Spontaneous emission (172 nm)	$Xe_2 \Rightarrow 2Xe$
Spontaneous emission	$Xe_1 \Rightarrow Xe$

The simulation model based on the fluid equations calculated the time-dependent population densities of all neutral and charged species in the plasma. Energy balance equations are solved for the electrons while the momentum conservation is considered via the transport equations using the drift-diffusion approximation. The set of the coupled rate equations is discretized by the Galerkin method built into the COMSOL Multiphysics environment, which is further solved by the solver PARDISO of COMSOL, taking the initial time step of 10^{-13} s.

3 Result and Discussion

The simulation analysis has been performed at different gas pressures. The typical V-I characteristics of the simulated co-axial xenon excimer source at 100 mbar pressure is shown in Fig 1. It has been observed that the peak current is obtained at the rising edge of the applied voltage pulse. The current reaches its maximum value at a voltage of 2.6 kV. After reaching the maximum value, the current starts decreasing due to the opposing electric field created by the charge carriers, accumulated on the dielectric surface and forming a pulse having a width of ~200 ns. The transit time of an electron is primarily determined by the current pulse width. During the rising phase of the applied voltage pulse, the ionization mechanism progresses gradually

mainly by the direct ionization of the Xe which is governed by the Townsend ionization coefficient. As the density of the metastable Xe atom in the discharge gap increases, a sudden transition in the ionization occurs; from direct ionization to stepwise ionization (i.e. ionization of the metastable Xe). This results in a higher peak current. In the subsequent pulse, metastable Xe density is higher which results in a higher current due to stepwise ionization. Hence, more current is obtained during the rising phase of the subsequent applied voltage pulse.



Fig 1. V-I characteristics of the simulated xenon excimer source having gas pressure of 100 mbar.

The spatial distribution of the electron density at the end of the voltage pulse is shown in Fig 2 for the Xe gas pressure of 100 and 150 mbar, respectively. The result shows that at the end of the pulse ($\sim 1 \mu s$) electron density is maximum near the cathode which is found to be $\sim 7 \times 10^{18} m^{-3}$ and $1.8 \times 10^{19} m^{-3}$ at 100 and 150 mbar, respectively. A high electron density region is formed near the cathode. As the pressure increases, electron density increases and the area of the high electron density region is reduced i.e. plasma is more constricted near the cathode at higher pressure.



Fig 2. Electron density surface plot in the Xenon excimer source with applied negative voltage pulse of amplitude 5 kV and frequency 25 kHz for Xenon pressure of (a) 100 mbar (b) 150 mbar.

Figure 3 illustrates the density of the xenon excimer Xe_2 in the gas gap region of 4 mm at different instant time as mentioned in figure for the case of 100 mbar and 150 mbar, respectively. It has been observed that the higher concentration of Xe_2 is obtained near the cathode for the gas pressure of 150 mbar. This is because of higher electron density near the cathode that results the larger number of excitations of xenon atom which ultimately formed the xenon excimer Xe_2 .



Fig 3. Spatial evolution of the Xe_2 excimer density at different instants of the time of the first pulse for the case of (a) 100 mbar and (b) 150 mbar.

4 Conclusion

The simulation has been performed using the 1-D fluid model in the COMSOL Multiphysics software for the discharge characteristics of the single barrier co-axial xenon excimer source. The simulation has been carried out for an excimer ignition using negative voltage pulse of magnitude 5 kV at a repetition rate of 25 kHz considering two sets of operating gas pressures of 100 and 150 mbar. The spatio-temporal characteristics of the Xenon excimer radiating 172 nm was investigated. It has been observed that the concentration of Xe_2 is higher near the cathode due to the availability of energetic electrons. The energetic electrons enhanced the density of the excited Xe_1 atoms via electron impact excitation, and the higher concentration of Xe_1 facilitated their conversion into the Xe_2 excimers. The higher pressure of xenon i.e., 150 mbar resulted in higher concentration of Xe_2 excimer which emits the radiation of wavelength at 172 nm.

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