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Molecular level mechanisms in microplasmas at cryogenic temperatures

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Microplasmas at cryogenic temperatures are known for showing neutral gas dependent characteristics, owing to their weakly ionized nature. An example of such plasmas is the dielectric barrier discharge (DBD) plasma, both in the planar, as well as in the jet configuration at cryogenic temperatures [1,2]. These plasmas show several interesting phenomena such as self-organized patterns, varying electron coupling parameter, and variable discharge modes with the change in gas temperatures (T_g) [1,2]. It is understood from the literature that for $T_g < 50$ K, the electron coupling parameter ($\Gamma_{ee} = \frac{e^2}{4\pi\varepsilon_0 a_e k_B T_e}$, where a_e is the mean inter-particle separation and T_e is the electron temperature), defined as the ratio of the mean potential energy to the mean kinetic energy of the electrons, increases rapidly. These observations intrigue one to unravel the underlying physical phenomena in these plasmas, especially the ion dynamics, which has not been studied in greater detail, experimentally. Further, the planar geometry of a DBD acts as a confinement to the plasma, which may have significant effects on the plasma dynamics, as observed for the confined neutral gases [3]. To understand these problems from a molecular standpoint, we employ molecular dynamics simulations in this work.

Unlike the fluid model, which is vastly used to describe the microplasmas, this work considers the contributions of each particle (ions and neutrals) to understand the dynamics and energetics of the plasma. The effect of the electrons is only considered through the shielding mechanism, accommodated in the Yukawa potential which guides the ionic interactions. The model is tested for different ionization fractions, ranging from 10^{-2} to 10^{-6}. The neutrals are assumed to be interacting through the Lennard-Jones potential, whereas the ion-neutral interactions are modeled by an effective potential [4].

In the first phase of the study, He gas molecules are distributed randomly in a simulation box having dimensions 150^3 nm^3 with periodic boundary conditions. The initial velocity distribution is chosen as a Gaussian type with the mean at the set value of T_g. Six values of T_g are chosen such as 30, 40, 50, 70, 100 and 150 K, with the initial gas pressure of 1 atmosphere. The gas particles are coupled to a Nose-Hoover thermostat to maintain the set T_g, thus forming an NVT ensemble with the number of molecules, volume and temperature being constants. The gas is thermalized for ~ 10 ns for each value of T_g such that the gas attains thermal equilibrium and the system converges. The He^+ ions are then distributed randomly with an initial velocity distribution of Gaussian type corresponding to the value of T_g. The ions form an NVE ensemble, with their number, volume and energy being the constants. It is assumed that the ion temperature (T_i) ~ T_g. Thereafter, the system is allowed to evolve and the radial distribution function (RDF), mean squared displacement (MSD), velocity distribution and images are obtained at required time steps for both the ions and neutrals. From the initial results, it is found that the ions show an initial heating effect for a few ns, and cool down as they interact with the neutral molecules. To further investigate the effect of such heating on the neutrals and the nature of interaction among the various species, both the neutrals and ions are allowed to evolve in an NVE ensemble. The thermostat coupled with the gas is turned off post thermalization for this procedure.

To understand the effect of confinement due to the electrodes, a confined system is chosen where the walls act as the thermal reservoir and both the gas and the ions are allowed to evolve in an NVE ensemble. An example of such a system is shown in Fig. 1. A detailed description on this section will be found in the conference.

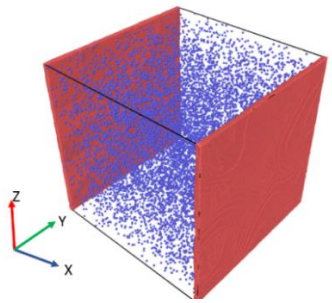

Fig. 1 Snapshot of the confined simulation system. Brown colour shows the walls and blue dots show He atoms.

References

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