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Investigating cryoplasmas through molecular dynamics simulations

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Helium plasmas at atmospheric pressure are widely studied employing various experiments and find applications in medicine, biology, and surface modification of materials. At room temperature (300 K), these plasmas exhibit strong ion coupling, ion heating and distinctive ion-neutral structure depending upon the ionization fraction (ion density/total density), which may vary from 10^{-1} – 10^{-8} [1]. These properties and underlying processes can be investigated using molecular dynamics (MD) simulations.

Accurate inter-particle potentials are crucial for MD simulations. For the ionic interaction, we compared Coulomb and Yukawa potentials for helium plasmas (ionization fractions = 10^{-1} - 10^{-6}) at 300 K. Yukawa potential accounts for the electron screening provided by the background plasma electrons. The screening constant is given by, $\kappa = \sqrt{n_e e^2/\epsilon_0 k_B T_e}$, where n_e is the electron density, e is the elementary charge, ϵ_0 is the permittivity of the free space, T_e is the electron temperature, and k_B is the Boltzmann constant. It is concluded that the effect of the electron screening is significant for the strongly ionized plasmas in terms of the ion temperatures and ion coupling parameter (mean ion-ion potential energy/mean ion kinetic energy). Figure 1 shows the maximum ion temperatures for both potentials for different ionization fractions. It is observed that the ion heating is limited for the Yukawa potential for strongly ionized plasmas. For weakly ionized plasmas, electron screening primarily affects ion-neutral structure [1]. Ion-neutral interactions are modeled using the charge-induced dipole potential.

To extend the MD study to the cryogenic gas temperatures (below 300 K to 30 K), the moderate and weakly ionized (ionization fraction = 10^{-3} – 10^{-6}) helium cryoplasmas are investigated in this work using Yukawa potential. The values of κ and ionization fraction are acquired from the experiments carried out in the cryoplasma experimental set-up (employing dielectric barrier discharge (DBD)) developed in our lab at IIT Kanpur. The plasma is generated at different gas temperatures from 300 K to 30 K, and characterized in terms of n_e, T_e, digital images and intensities of the emission spectra. Such a characterization is helpful in understanding the gas temperature dependent macroscopic properties of the plasma. The influence of the applied voltage and frequency on the plasma properties are also examined. It is expected that a lower gas temperature and optimum experimental condition would result in strongly coupled ions in the plasmas even for a lower value of ionization fraction. In parallel, the MD simulations will help in understanding the ongoing microscopic processes at very short timescales (~ a few ns) in terms of the temperature evolution of ions, the radial distribution function, and transport coefficients of the plasma. At lower gas temperatures, the plasma is expected to be thermally stable (reduced thermal fluctuations in plasma parameters) and ordered in structure, as observed for the neutral gases [2,3]. Therefore, the experimental results combined with the simulations will provide important information regarding the plasma dynamics, energetics, structure and stability at low gas temperatures.

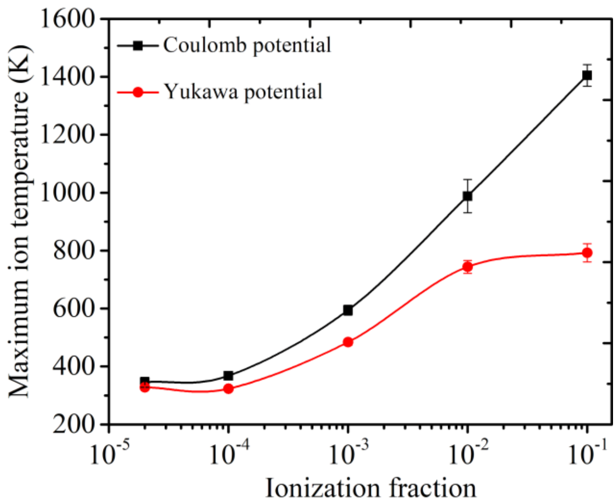

Figure 1. Maximum ion temperatures for Coulomb and Yukawa potentials for different ionization fractions.

References

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