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Molecular dynamics simulations of gas and plasma transport under confinement and in the cryogenic limit

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Molecular dynamics simulation is expected to be an efficient tool to investigate the transport, dynamics, structures, and energetics of weakly ionized cryoplasmas. These plasmas are mostly generated in the cryogenic temperatures (4 - 150 K), and atmospheric pressure, using dielectric barrier discharge (DBD). The plasma properties such as, electron temperature and density, structural properties, and plasma chemistry, have been observed to be influenced by gas temperatures in earlier experiments [1,2]. However, the molecular-level mechanism of gas-plasma interactions involved in the aforementioned observations is yet to be understood. Furthermore, being microplasmas, the plasma behavior is also expected to be influenced by the confinement caused by the walls of the DBD and the experimental chamber. These plasmas are expected to achieve correlated and strongly coupled behavior, similar to those found in the exoplanets. In this context, we propose to present an overview of equilibrium (simulations carried out at constant temperature) and non-equilibrium (simulation carried out at variable temperature) molecular dynamics simulations of confined He gas and He cryoplasma.

In this three-phase study, the first study focuses on the equilibrium transport properties of confined He at different set temperatures, ranging from 30 K to 150 K. The effect of the walls causes the reduction in the values of the transport coefficients such as, self-diffusion coefficient (D) and thermal conductivity (λ) along the direction of confinement ($D_\perp$ and $\lambda_\perp$) [2]. The directional values of D (as seen in Figure 1) have been computed from the linear regime of the respective mean squared displacement graphs, whereas, the values of λ have been computed using the simulated values of D and non-equilibrium method. The obtained values are compared with the values simulated for bulk He gas, to estimate the effect of the confinement. To validate the simulation results for the bulk gas, the results are further compared with those obtained from quantum mechanical calculations and literature.

After characterizing the confined gas in terms of its transport coefficients, non-equilibrium simulations are carried out to understand the metallic wall assisted collisional cooling, which is the cooling mechanism of the neutral gas in the cryoplasma experiments. For different wall temperatures ranging from 30 - 100 K, cooling curves are obtained for He, initially maintained at 150 K and atmospheric pressure. The cooling rates are calculated for different temperature gradients (ΔT), which is defined as the temperature difference between the initial gas temperature and wall temperature. These curves indicate the ΔT dependence of heat transfer mechanism involved in the wall assisted cooling. Furthermore, the effect of presence of a secondary gas (Ne and Ar) in equal proportion as He on the cooling rate of He is investigated. Effect of mass of the secondary gas on the heat transfer between the metallic walls and He is expressed mathematically. Lastly, near-wall activity of He in the non-equilibrium condition is understood in the presence of the secondary gas, which contributes towards the gaseous structure during the cooling process [3].

Finally, in the third phase, He cryoplasma is simulated by considering various inter-species interactions, such as, interactions among the charged species, gas-plasma interactions, gas-gas interactions, gas-surface interactions and plasma-surface interactions. Thereafter, the energies and densities of various plasma species are calculated at different set temperatures. Upon validating the simulation results with comparison with the available experimental results from literature, the diffusion coefficients of the plasma species are determined and presented with varying temperature.

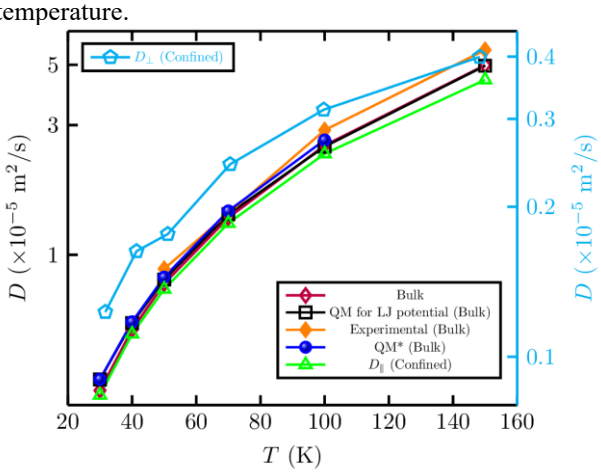

Figure 1. Directional values of self-diffusion coefficient (D) for the confined system at different temperatures. The results are compared to those for the bulk system, obtained from simulations, quantum mechanical calculations (QM), and literature (experiments and QM*).

References:

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[3] S.S.Mishra and S.Bhattacharjee (Submitted).

[4] S.S.Mishra and S.Bhattacharjee (Under preparation).