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Effect of Confining Metal Walls on The Helium Gas Dynamics at Low Temperature: A Novel Approach to Understanding Cryoplasmas Employing Molecular Dynamics Simulation

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In the noble gas family, helium (He) is the least understood element, owing to its peculiar properties, particularly at temperatures below room temperature. Due to its light mass and small size, the onset of quantum properties takes place at relatively higher temperatures (~ 150 K), compared to the other gases of the family. Further, the expression of the quantum nature of the gas is highly dependent on the observable which is to be measured [1]. These phenomena often restrict the thorough physical description of the gas at low temperatures (below 150 K), as drawing a boundary between quantum and classical regimes of He gas becomes critical. However, the understanding of the physical processes involved in the gas dynamics in these temperatures is crucial for elucidating the dynamics and energetics of cryoplasmas. Cryoplasmas are microplasmas generated at cryogenic temperatures (below room temperature to liquid He temperature) and near atmospheric pressure. Owing to the weakly ionized nature of these plasmas, the role of neutral ambient gas is vital in predicting plasma behavior. Furthermore, the gas – surface interactions in such plasma systems are equally important in determining the structural and dynamical properties of the plasma, as these interactions explicitly affect the neutral gas dynamics [2]. Therefore, we employ classical molecular dynamics (MD) simulations to study the energetics and transport phenomena in pure He gas using Lennard – Jones (LJ) potential, in the temperature range of 150 K to 30 K and at atmospheric pressure. The dimension of the gas region is $600\times600\times600$ angstrom^3. The study is twofold. Initially, the gas is studied as a bulk system under NVT ensemble (particle number (N), the volume of the gas (V) and gas temperature (T) are constant), in which the gaseous system is coupled with a Nose – Hoover thermostat [3] to maintain the set gas temperature (T). In this exercise, various transport properties like self-diffusion coefficient (D) and thermal conductivity (λ) are calculated from the simulations. These values are then compared with the available experimental and quantum mechanically calculated data to ascertain the correctness of the modeling and visualize the emergence of the quantum nature of the gas [4]. In the latter part, a pair of metallic walls, each of 10 angstrom thickness is introduced in both the positive and negative X direction of the gas region studied earlier. The walls are made up of Fe atoms and modeled using embedded atomic model (EAM) potential. Further, the gas – wall interactions are designated by Morse potential [5]. Such a gaseous system is termed as a confined system. All the simulations are performed using LAMMPS [6].

A comparative study of the potential energy of the gas in both bulk and the confined system can enlighten the roles of gas – wall interaction and long - range forces in system energetics at low temperatures. Thereafter, the effect of wall mediated collisions on the transport mechanism of the gaseous system in the confined case is understood by comparing its velocity auto-correlation functions (VACF) and mean squared displacement (MSD) curves with respect to the reduced time ($t^* = t$ /characteristic time for He) with the bulk system counterparts.

Fig.1. shows the comparison of MSD versus t^* curves for both systems. The comparison clearly indicates the reduced mobility of the gas molecules in the case of a confined system compared to the bulk system [7,8]. Such increase in mobility can be attributed to the combined effect of the increase in collision frequency and the effect of long – range attractive forces. In addition, this curve can act as a master curve to determine the transport coefficients (D and λ) for the system, which upon comparison with those of bulk system can foretell about the degree of reduction in the mobility of the gas molecules due to the presence of the boundary in the microscopic scale.

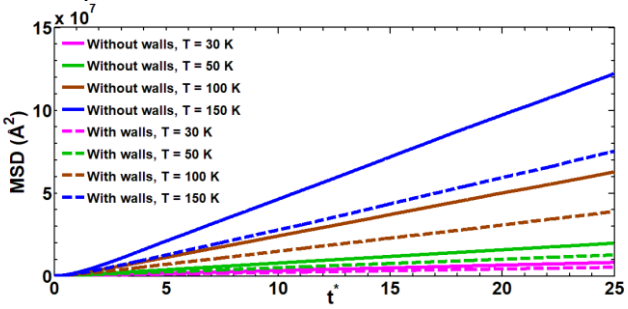

Figure 1. MSD versus t^* curves for both systems.

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