

## Molecular dynamics simulation of collisional cooling of He and its binary mixtures with Ne, Ar, Kr and Xe in Nose-Hoover thermostat for creating strongly coupled cryo-plasmas

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Cryo-plasmas are micro-plasmas created in extremely low temperatures (below room temperature to 4K) and usually at atmospheric pressure. They provide an excellent platform to investigate physics of strongly coupled systems, where the plasma in the ambient gas can be taken to extremely low temperatures, and further dust added to them. Both these effects are together expected to increase the coupling parameter (ratio of the typical potential energy to kinetic energy of nearest neighbors) significantly and take it to regimes not investigated earlier. In these plasmas, neutral gas temperature dependent dynamics control the energetics of electrons and ions, owing to their weakly ionized nature [1]. Most of the studies in this field are focused on the production and properties of pure He cryo-plasma [1,2]. The first step of generating such a plasma is to cool the gas inside a vessel connected to a cryostat. One of the most significant findings from such studies, is the dependence of electron density, temperature and hence the particle coupling parameter on neutral gas temperatures. Such a dependence primarily originates from the inter-particle interactions in neutral gas [1].

In order to be able to predict how the interactions of neutral gas molecules control the plasma dynamics, two studies are vital: (i) a proper knowledge of the correct interaction potential acting between the gaseous atoms, and (ii) the efficiency of collisional cooling of gas atoms and eventually the cooling of plasma electrons (and ions) through interaction with neutral atoms in such low temperatures (~10K). Though, the Lennard-Jones (LJ) (6-12) potential is conventionally used to model real gases and fluids [6], there arises several discrepancies at cryogenic temperatures, due to the emergence of quantum effects, which puts the validity of such potential under scrutiny, in the aforementioned temperature range.

In order to investigate the cooling process, the effect of gas mixing of He with other gases such as Ne, Ar, Kr and Xe, a 3D molecular dynamics simulation has been set up, using the LAMMPS package [3]. The monatomic gases are chosen based upon their polarizability, atomic radius and mass. The considered simulation box has periodic boundary conditions in all directions. To replicate the experimental style of cooling, the experimental chamber has been assumed to be a thermostat. For this purpose, Nose-Hoover type of thermostat has been used, which gives rise to a statistical canonical ensemble [4]. The temperature damping parameter is set to be 0.1ps for all the processes. The cooling process is carried out starting from 300K to 10K, with a starting pressure of 1atm and a time step of 1fs. The chosen pair potential (Lennard-Jones), has the form:  $\phi_{LJ}(r_{ij}) =$

$4\epsilon \left[ \left( \frac{r_{ij}}{\sigma} \right)^{-12} - \left( \frac{r_{ij}}{\sigma} \right)^{-6} \right]$ ; where,  $\epsilon$  is the interaction strength and  $\sigma$  is the distance parameter. To guide the interactions between unlike atoms, two types of combining rules are used, such as Lorentz–Berthelot (LB) and Fender–Halsey (FH) [7]. For the binary mixtures, the gas mixing ratio is taken in 1:1 proportion.

The initial simulations have been carried out for a pure He system. The gas particles are cooled starting from 300K to 10K. The speed (velocity) distribution functions are obtained for 200K, 100K and 10K respectively. The velocity distributions are acquired for an equilibration time period of 20ns, with 2ns intervals. Final distribution plots are generated by using time averaging method. Figure 1 shows the comparison of obtained velocity distributions from MD simulations, with the theoretically predicted Maxwell-Boltzmann distribution curves. The excellent agreement between the simulation and theoretical results, assures the successful implementation of the simulation system.

In the conference, the cooling rate of such pure He system and the mixtures will be presented. The effect of mass, size and interaction strength of secondary gas on the cooling rate of He are to be discussed. The performance of the LJ potential, and both the mixing rules, will be ascertained by comparing the time dependent transport properties with the available experimental results [5,6]. Finally, the onset of quantum effects will be investigated, which is estimated by comparing the inter-particle distance and the de-Broglie wavelength.

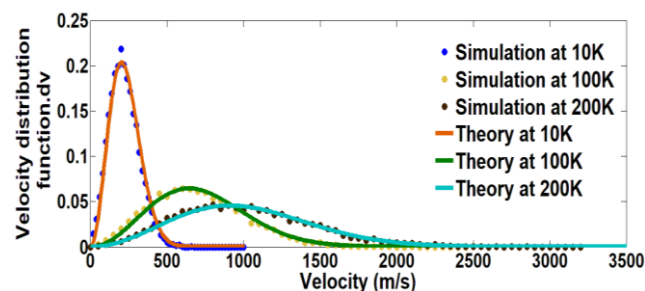


Fig 1. Velocity distributions at various temperatures

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