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MD simulations of pure inert gases in 2d and 3d and their mixture in 3d

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Abstract
The present work consists of the MD simulation of the Ar system in two dimension and in three dimension and Ar-Kr binary mixture in three dimensions by using Lennard-Jones Potential using periodic boundary condition through LAMMPS code and study its static properties. We have analysed the liquid structure in both the cases by looking at radial distribution function.

Keywords: MD simulation, LAMMPS, Lennard-Jones, Radial distribution function

1. Introduction
The invention of the computer has made simulations of different materials in different states possible. Over the years, a lot of theortical and experimental studies have been carried out by scientists to study the properties of the materials when they undergo a phase change [1]. The first successful attempt was made to solve the equations of motion for a set of Lennard Jones particles by Rahman in 1964 in which a system of 864 particles interacting with a Lennard-Jones potential and obeying classical equations of motion was studied on a digital computer (CDC 3600) to simulate molecular dynamics in liquid argon at 94.4 K and a density of 1.374 g cm^{-3}, and in this case the pair-correlation function and the constant of self-diffusion were found to agree well with experiment [2]. In this paper we present the MD simulation of the Ar system in two dimension and in three dimension and Ar-Kr binary mixture in three dimensions by using Lennard-Jones Potential using periodic boundary condition through LAMMPS code [3] and study its staticc property. We have analysed the liquid structure in both the cases by looking at static properties, which characterize the local structure of the fluid. We studied the structural properties of the 3D and 2D dense fluids using the radial distribution function g(r).

1.1 Binary Mixture
A binary liquid mixture or a two-component fluid can be made by mixing liquid with a liquid, gas with a gas, dissolving a solid in a liquid or by mixing a liquid with a gas that dissolved easily in a liquid [4]. The study of these liquid mixtures involves complications. Composition is the basic property of the single-phase liquid mixture; A two component fluid is a system comprise of N1 particles which can be atoms or molecules depending upon the type of component each of which is having mass m1 and N2 particles of mass m2 each and having volume V. The most important parameters regarding the composition of the two-component liquid mixture are the mole fraction N1/N which is usually referred to as the concentration of N1 in the mixture. Second parameter is the mass fraction m/Ξmi. The other important parameters are mass density mi/V and number density ni/V. In case of the binary fluid mixtures it is quite usual to express concentration only in terms of mole fraction where c is mole fraction of the one component and other can be considered as (1- c). The effects of the variations in concentration, mass and size along with the interaction among the particles of the binary fluid mixture play an important role in the study of the transport properties. In our present work we have considered the two species which differ only in their masses.

2. LJ Parameters for Simulation of Ar, Kr and their Mixture

In the present work, we are studing the molecular dynamic simulations of Ar, Kr and Ar-Kr binary mixture using the Lennard-Jones Potential so we need to know the Lennard-Jones parameters for the liquid Ar, Kr and Ar-Kr mixture. Typically, physical quantities measured in MD simulations are represented in dimensionless form in reduced units. Dimensionless units provide several computational benefits, such as numerical values close to unity with the equations of motion without large exponents of the coefficients involved. Also, as stated earlier the biggest benefit of using dimensionless units is that a single model represented in dimensionless units can be scaled for different problems. Using σ, m, and ϵ as units of length, mass, and energy respectively, dimensionless quantities for length, energy, time, pressure, and density are defined as: [11]

Table 1: LJ parameter for Ar, Kr and Ar-Kr mixture in real units

S. No.	Quantity	LJ parameters for Ar	LJ parameters for Kr	LJ parameters for Ar-Kr
1	length [10^{10} m]	$\sigma = 3.4$	$\sigma = 3.64$	$\sigma = 3.52$
2	energy [10^{21} J]	$\epsilon = 1.65$	$\epsilon = 2.30$	$\epsilon = 1.95$
3	mass [10^{26} kg]	$m = 6.64$	$m = 13.92$	

Table 2: LJ parameters for Ar, Kr and Ar-Kr mixture in reduced units

S. No.	Quantity	LJ parameters for Ar	LJ parameters for Kr	LJ parameters for Ar-Kr
1	length	$\sigma^* = 1$	$\sigma^* = 1.067$	$\sigma^* = 1.0332$
2	energy	$\epsilon^* = 1$	$\epsilon^* = 1.394$	$\epsilon^* = 1.1806$
3	mass	$m^* = 1$	$m^* = 2.096$	

- **length:** $v \rightarrow v\sigma$
- **energy:** e $\rightarrow e\epsilon$
- **time:** t $\rightarrow t(m\sigma^2/\epsilon)^{1/2}$
- **pressure:** p $\rightarrow p\sigma^3/\epsilon$
- **density:** $\rho \rightarrow \rho\sigma^3/m$
- **velocity:** $(\epsilon/m)^{1/2}$
- **force:** ϵ/σ
- **temperature:** ϵ/k

So, the LJ parameters of Argon required for its MD simulation in real as well as reduced units have been shown in table 1 and 2 [12]. The density in reduced units which is given as $\rho^* = \rho\sigma^3/m$. For the current choice this becomes $\rho^* = 0.82$. The cross-interaction parameters between Ar and Kr ar calculated from the simple Lorentz- Berthelot rules [4]:

$$\epsilon_{ij} = (\epsilon_i \epsilon_j)^{1/2} \quad (1)$$

and

$$\sigma_{ij} = \frac{\sigma_i + \sigma_j}{2} \quad (2)$$

2.1 Physical Description of the Properties

Physical properties which we are going to look at, namely Radial distribution function will be calculated seperately for pure Ar in two dimension and three dimension and for Ar-Kr binary mixture in three dimensions.

3. Molecular Dynamic Simulation of Argon System in Two Dimension

Motivation here is to verify that the state of lowest energy for a two-dimensional Lennard-Jones solid is a triangular lattice rather than a square lattice. Here we tried to stimulate a 2D Argon system with an initial square lattice structure and the simulation is given a run of 1000000 timesteps.

Initialisation

We have initialised our simulation for the Argon system with 81 particles of mass m by taking parmeters of argon interacting via the Lennard-Jones pair potential. The potential was truncated at 2.5σ and then shifted. We chose the particles in a square lattice and chose the parameters in the lennard jones (lj) units. We distributed the velocities of the particles using gaussian distribution. Newton equation of motions were integrated using Verlets algorithm [13]. The periodic boundary conditions were imposed in the system. With the periodic boundary conditions, we have eliminated the surfaces and created a quasi-infinite volume/area to represent the macroscopic system more closely. We took the system in the NVE ensembles. After establising an equilibrium configuration, the MD runs were carried out for 1000000-time steps with $\Delta t^* = 0.005$ that correspond to about 2×10^{12} sec. The Input script used for this simulation is given later in the appendix 1. The starting configuration of the system is shown by x movie and V md tools in figure 1.

Equilibriation

Equilibrium is established if the system has settled to definite mean values of the kinetic and potential energies. To check the equilibriation phase of the system, we made sure that the after system has relaxed the system has reached a long-lived metastable state. The metastable state of the square lattice is the triangular lattice as visualised by x movie and V md and it is shown in the figure 2.

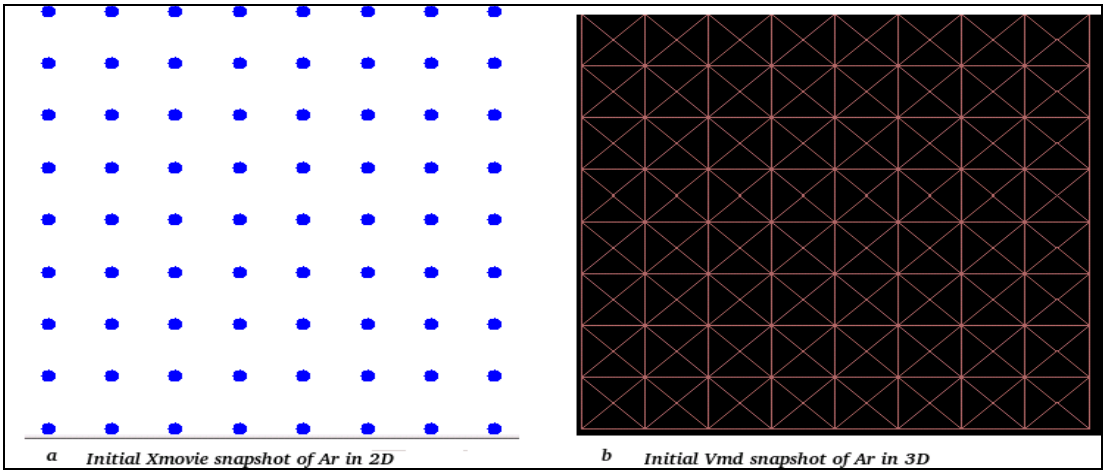

Fig 1: Initial X movie snapshot and V md snapshot for Ar system in two dimensions showing the initial structure of the system taken to be a square lattice

Production

After establishing the equilibrium configuration, we performed the production run to compute the physical quantities of interest such as radial distribution function g(r) (i.e. static property) and analysed them.

3.1 Radial Distribution Function

The radial distribution function has been plotted for an argon system in two di- dimensions in figure 3. A careful look at the g(r) versus r plots shows that the function g(r) becomes firstly zero at the short distances, where repulsive forces prevent overlapping of the molecules, when r is close to the collision diameter σ, g(r) increases rapidly to a maximum corresponding to the first peak implies that here the probability of finding a pair of atoms r distance appart is maximum. As r increases gradually, g(r) decreases, showing that the influence of the central atom is disappearing with increase in the distance. Here the first peak is at 0.52 across 1.14

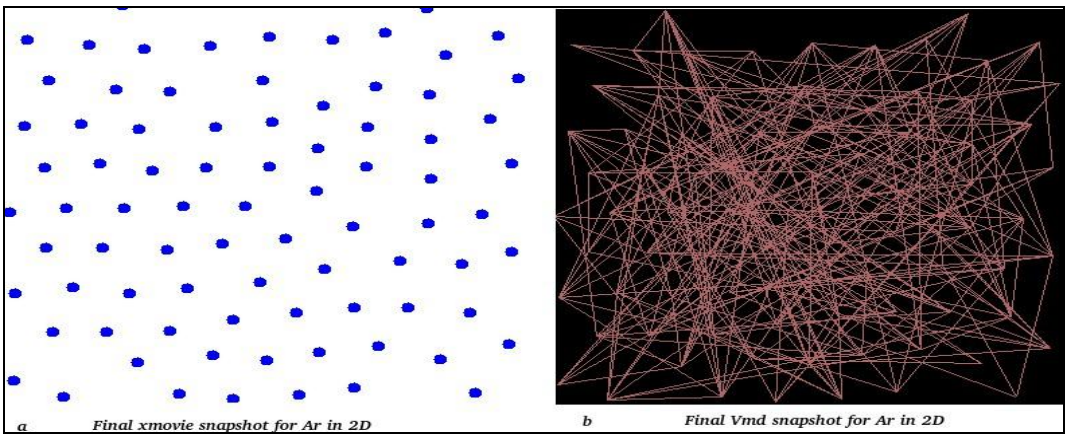

Fig 2: Final X movie snapshot and V md snapshot for Ar system in two dimensions showing that the metastable state of the system is indeed a triangular lattice.

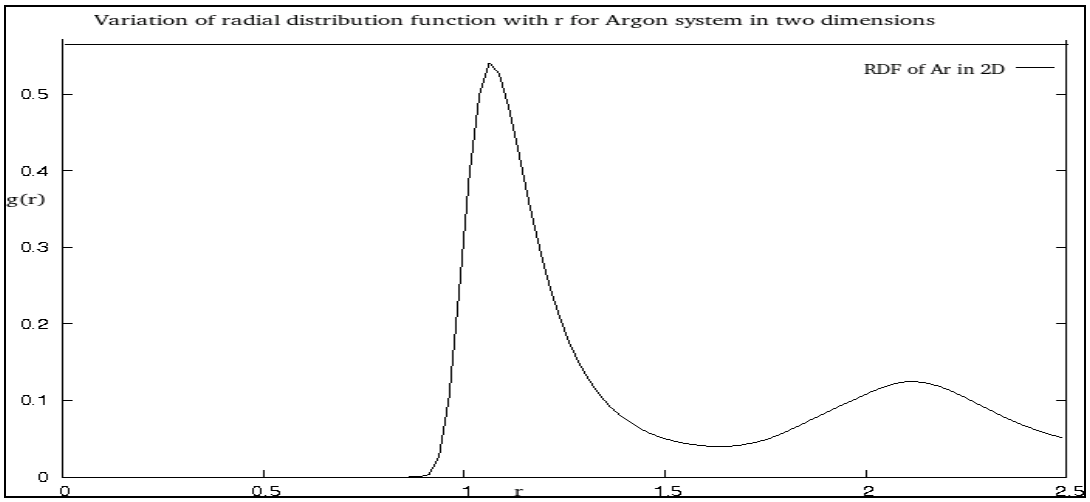

Fig 3: Plot of radial distribution function g(r) with r for Ar system in two dimensions

4. Molecular Dynamic Simulation of Argon in Three Dimension

Initialisation

In the initial configuration of a model dense crystal, atoms lie at the sites where the shortest interatomic distance (lattice parameter) is $2^{1/6}\sigma$, which correspond to a minimum of the Lennard Jones potential as shown in the figure 4.

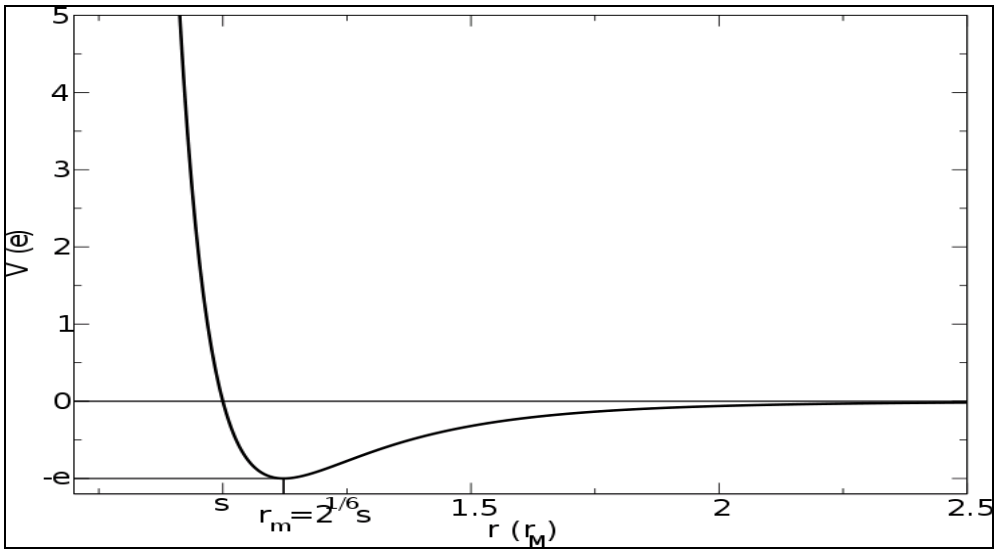

Fig 4: Lennard Jones potential [12]

The crystal is heated in the stepwise procedure i.e by increasing the temperature. For 3D system we have started our simulation with 4000 particles of mass m interacting via the Lennard-Jones pair potential. The Input script used for this simulation is given in the appendix 2 [3]. We chose the particles initially in fcc lattice. With the periodic boundary conditions, we had eliminated the surfaces and created a quasi-infinite volume/area to represent the macroscopic system more closely to real systems. The starting configuration of the 3D system is shown in the figure 5 in all the three planes.

Equilibriation

The most important point of the equilibriation phase is that the metastable state has the constant total energy after the system is relaxed. The evolution of the total energy, kinetic energy and potential energy is shown in the figure 6. We observe that the total energy remains constant and does not show a drift during the entire simulation. The Kinetic and Potential energies have changed initially at the equilibriation period but during the end of the simulations they oscilate around their equilibrium value.

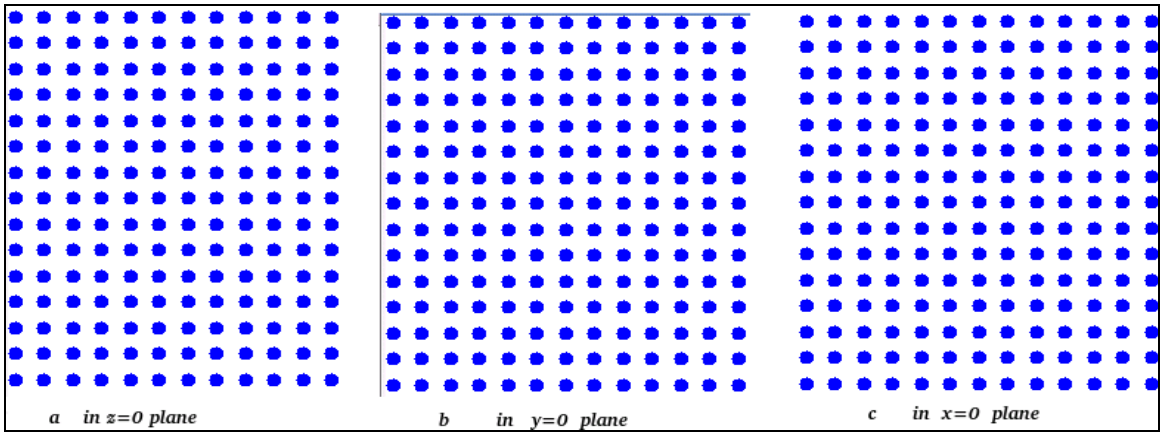

Fig 5: Initial x movie snapshot for Ar (a) in z=0 plane (b) in y=0 plane (c) in x=0 plane

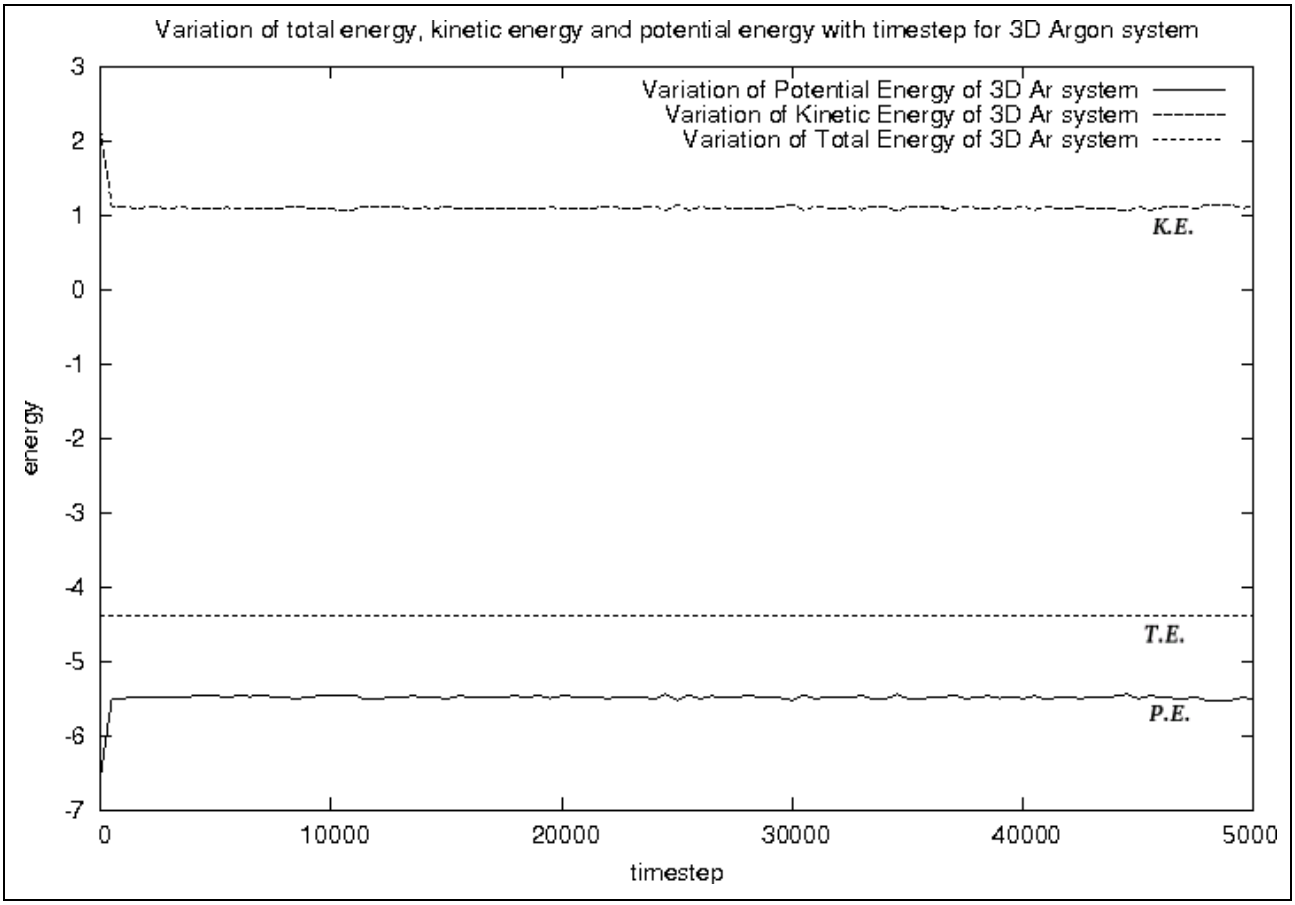

Fig 6: Variation of total energy, kinetic energy and potential energy with timesteps of Ar in three dimensions

4.1 Radial Distribution Function

The structure of the system in different states can be studied with the help of the RDF (radial distribution function). The RDF radial distribution function of an argon system in three dimension when timestep $t = 0$ is shown in the figure 8 at a reduced density of the $n^* = 0.82$. For the graph of the zero timestep the sharper peaks are observed showing a crystaline structure, also the value of the RDF is less then unity. This implies that the particles are localised and they are arranged in the regular manner, which is a signature of the crystalline structure of the system. The pair distribution function approaches unity as the temperature is increased, which means that the particles are distributed homogeneously inside the box and it shows a typical liquid structure. The figure 9 shows the plots of radial distribution function at different timesteps. Here the first peak of g(r) is at 3.0 at r = 1.1

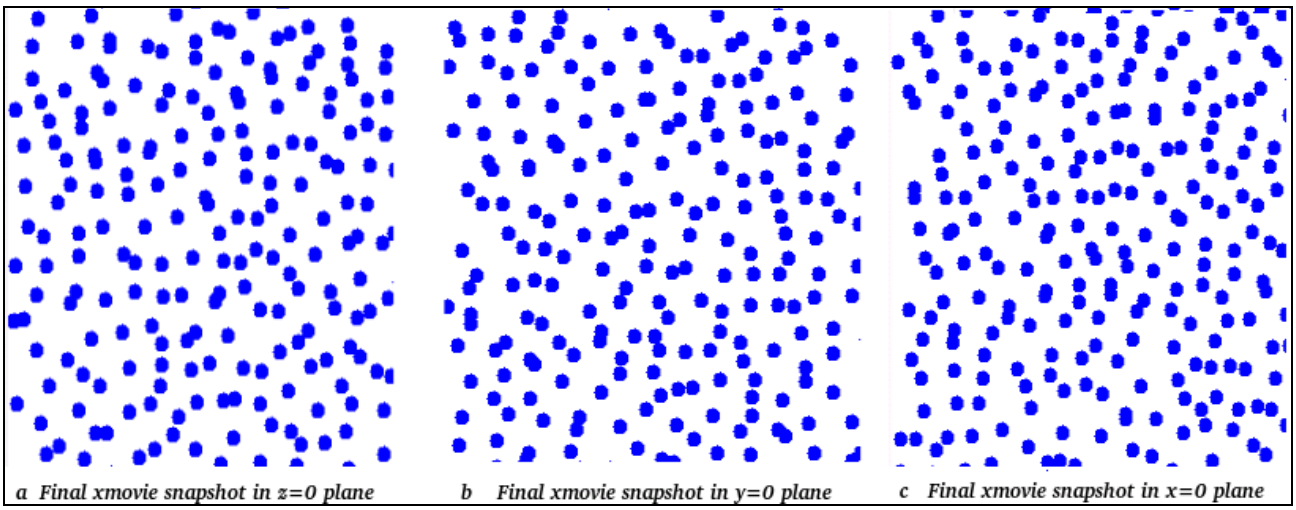

Fig 7: Final x movie snapshot for Ar (a) in z=0 plane (b) in y=0 plane (c) in x=0 plane

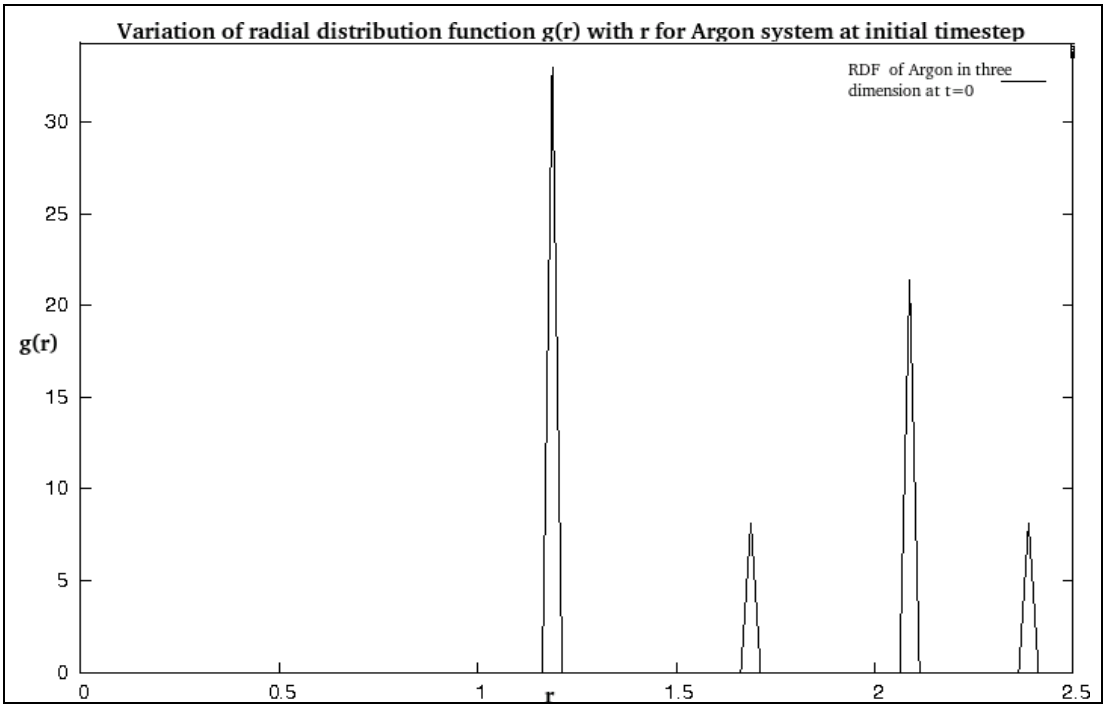

Fig 8: Plot between radial distribution function g(r) and r for Ar in three dimensions at t=0

5. Molecular Dynamic Simulation of Argon-Krypton Mixture

Initialisation: In this simulation of argon-krypton system we have 864 particles interacting via the Lennard-Jones pair potential. We have chosen the particles in a fcc lattice and the parameters in the lennard jones (lj) units. Newton equation of motions were integrated using Verlets algorithm [13]. The periodic boundary conditions were imposed in the system. The LAMMPS input script used for the binary mixture is given later in appendix 3 [3] The initial and final configuration of the Ar-Kr system can be seen in the using x movie in figure 10.

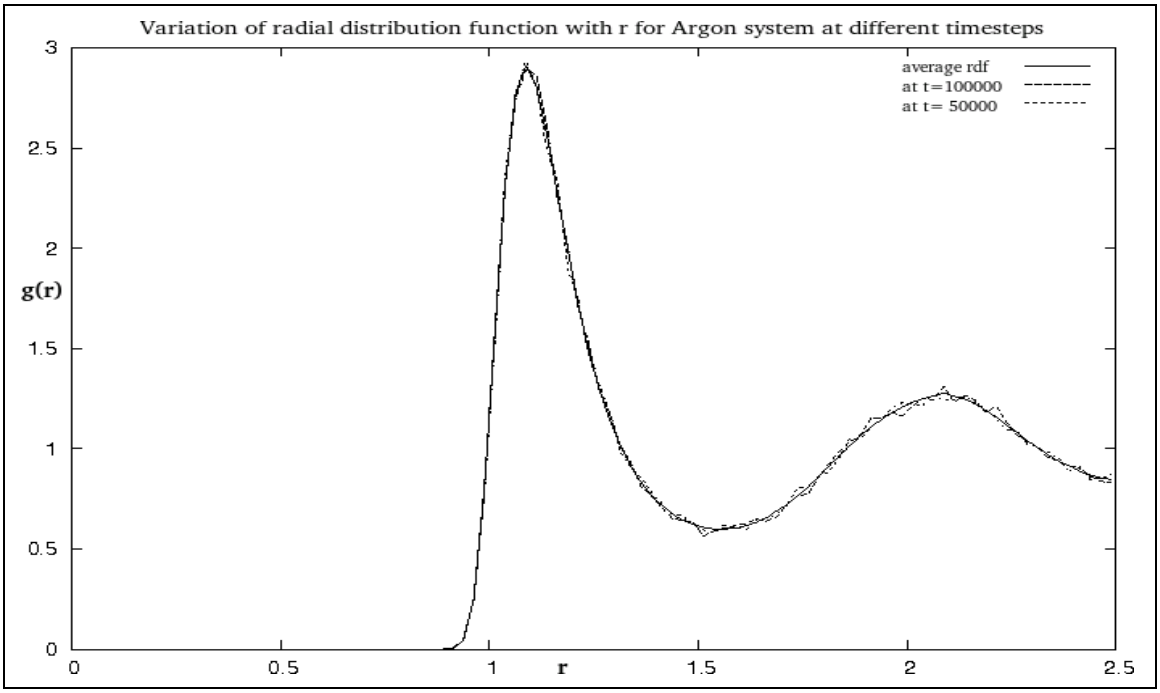

Fig 9: Plot of radial distribution function g(r) and r for Ar in three dimensions at different timestep

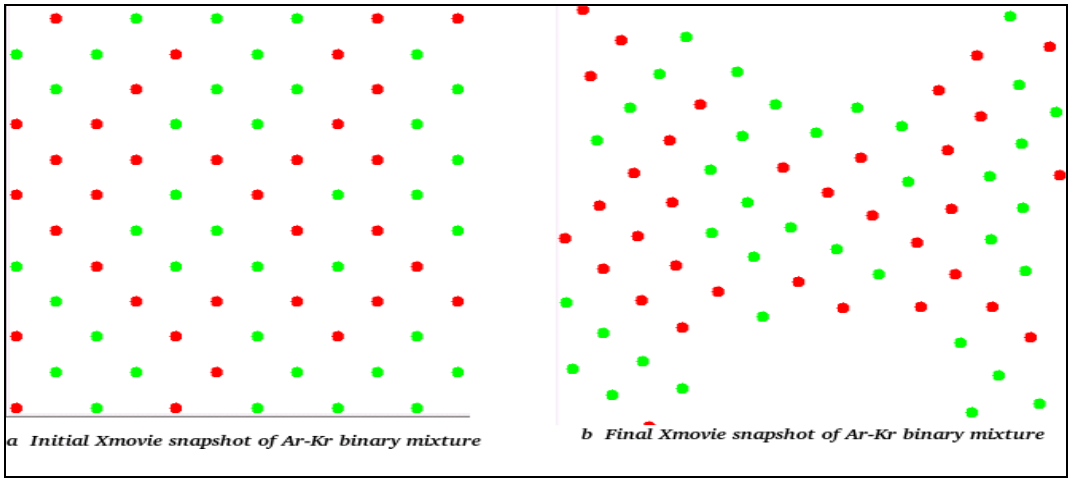

Fig 10: Initial and Final X movie snapashot for Ar-Kr binary mixture system in three dimensions

Equilibration

As we have done before, to check the equilibriation phase of the system, we made sure that the after system has relaxed the system has reached a long-lived metastable state. This was indeed the metastable state of the FCC lattice is the hcp lattice as seen in the figure 10. After reaching the metastable state the total energy of the system remained constant. The evolution of total energy, kinetic energy and potential energy is seen in figure11. We observe that the total energy remains constant and does not show a drift during the entire simulation. The Kinetic and Potential energies have changed initially at the equilibration period but during the end of the simulations they oscilate around their equilibrium value for all the systems.

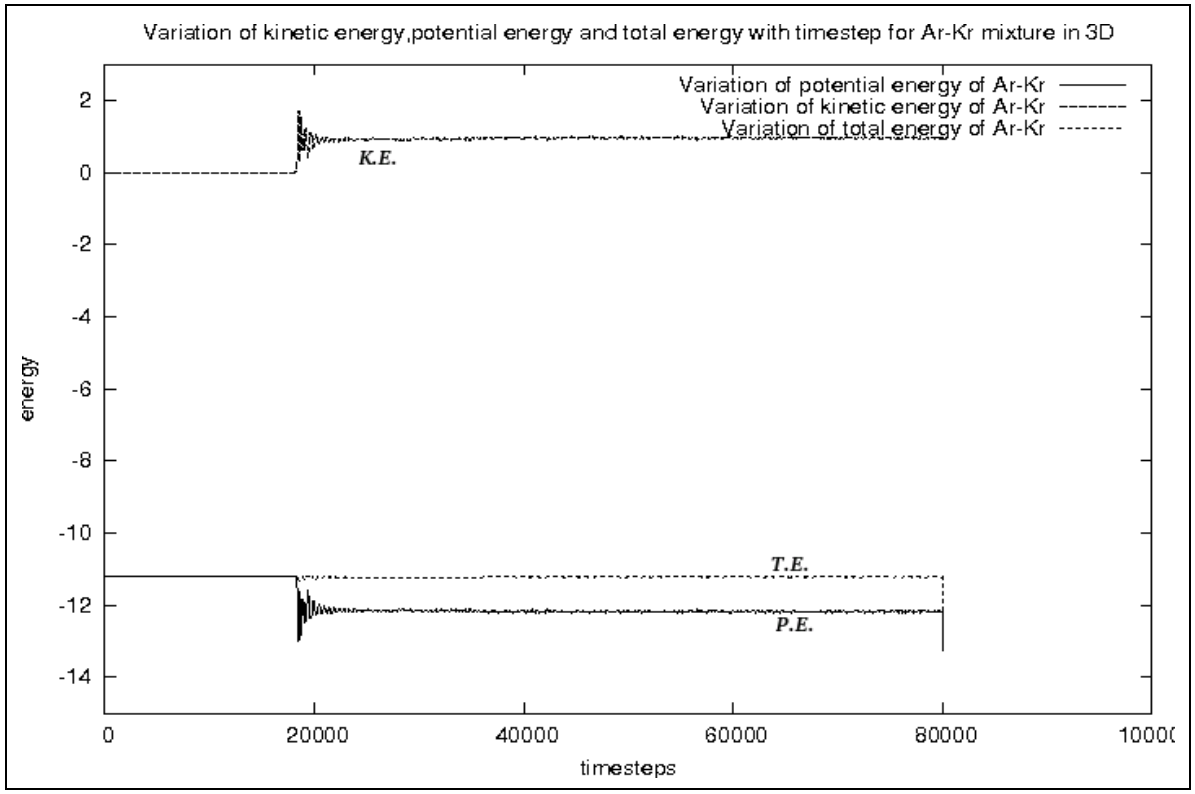

Fig 11: Variation of potential energy, kinetic energy and total energy with time for Ar-Kr binary mixture in three dimensions

Production

Similar to the 2D and 3D system discussed in the previous section, the actual com- putation of physical property of interest were made only after equilibrium had been established for all the systems.

5.1 Radial Distribution Function of the Ar-Kr Mixture

The figure 12 shows the radial distribution function for pure Ar, for the binary mixture of Ar and Kr at three different concentrations of 0.25, 0.50, and 0.75 and for pure Kr. The positions and heights of the first peaks reflect the magnitude of the LJ paramters σ and ϵ, respectively. That is, the smaller σ is, the closer molecules come, and the larger ϵ is, the more molecule come. The second peak of the g(r) is higher when the concentration of krypton is 0.75 followed by the height of the peak at a concentration of 0.5 and then by height of peak at concentration of 0.25 and it indicates that g(r) is increasing with the increase in concentration of krypton or decrease of concentration of argon. The first peak of g(r) for pure argon is at 3.0 which is lowest and for

the Ar-Kr mixture it lies at 4.5 and for pure krypton it is at 5.0 which is highest in all. This is the mixing effect. Thus the RDF of the Ar-Kr mixture is in between those of the Ar and Kr.

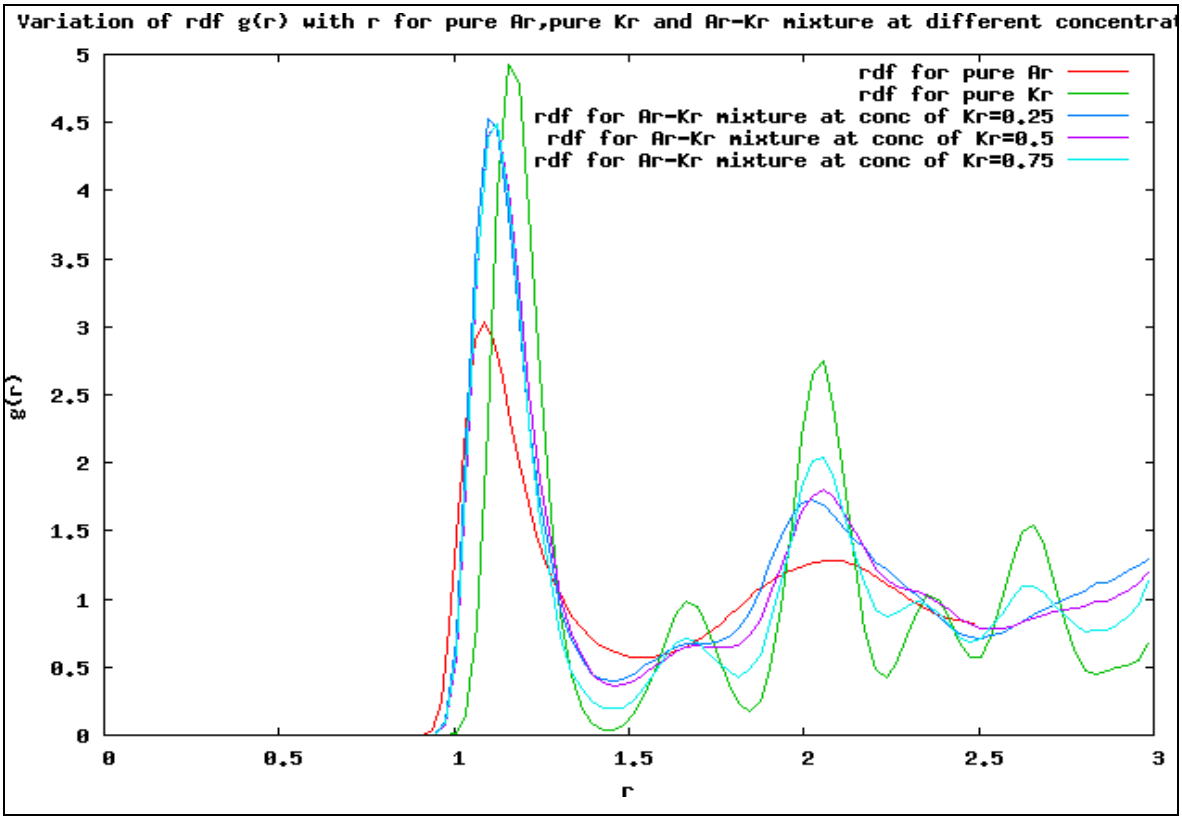

Fig 12: Variation of RDF with r for pure Ar, pure Kr and Ar-Kr mixture at different concentrations of Kr in mixture in three dimensions

6. Conclusion

We have investigated the behaviour of the pair distribution function and mean square displacement of the Argon system in two and three dimensions to look for distinctive structural features. It was found that the state of lowest energy for a two-dimensional Lennard-Jones solid is a triangular lattice rather than a square lattice and the metastable state of the fcc lattice was found to be the hcp lattice. The radial distribution function has a much higher peak in three dimensions than in two dimensions. We have investigated the behaviour of the pair distribution function and mean square displacement of the 3D argon-krypton mixture to look for distinctive structural features. The radial distribution function and mean square displacement plots for Ar-Kr mixture lies between pure argon and krypton and it varies with increase in concentration of krypton.

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