

# Project 07 - Molecular Dynamics Simulations Analysis

Simulation of Nanometric Systems - *Nanoscience and Nanotechnology* - 22/23

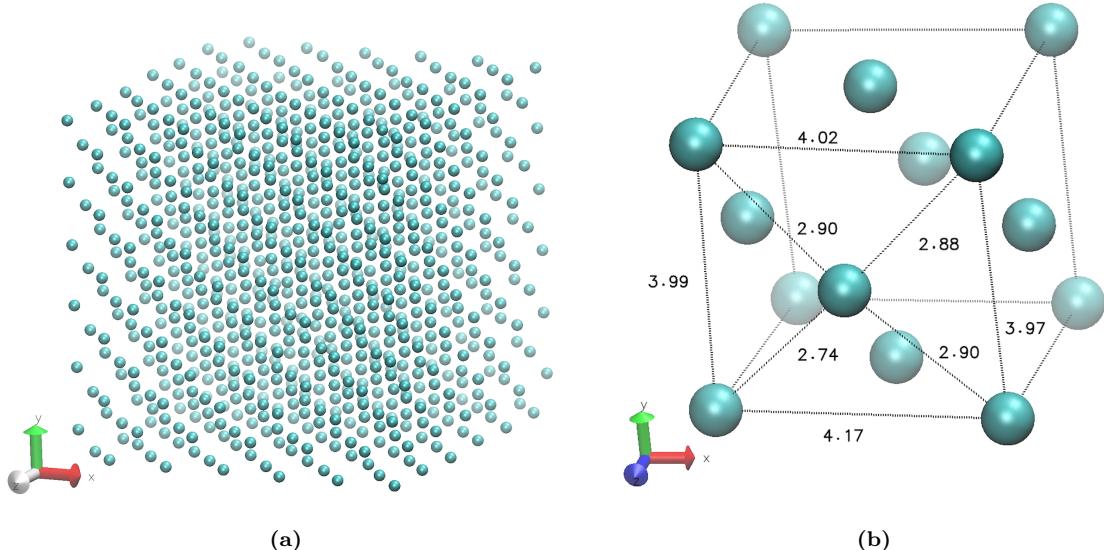
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In this project, we aimed to perform a simple molecular dynamics simulation and conduct a brief analysis of the results. The different files used can be found in my Github repository [1].

## 1 Initial Structure

To perform molecular dynamics simulations, we need four types of files:

- The input file for the simulation itself, in our case, it is an input file for NAMD.
- A file containing all the necessary information for each atom to properly simulate the nanoparticle, which is contained in “.psf” files.
- A file containing the coordinates of the atoms of what we want to simulate. In our case, we want to simulate a gold nanoparticle with an fcc structure and a separation between the first neighbors of approximately 3Å and a separation between the second neighbors of about 4Å, as we can see in Figure 1. This information is found in “.pdb” files.
- One or more files explicitly stating the “Force Field” to be used in the simulation, which tells us how each atom in the simulation will interact with its environment. This information will be in files with the “.inp” format. In our case, we will use a Lennard-Jones potential of type 12-6 between all the atoms.



**Figure 1:** **a**, Image of the entire structure. **b**, Section of a part of the structure where only the unit cell is visible, and the fcc organization with some of the bonds drawn can be appreciated.

## 2 Simulations

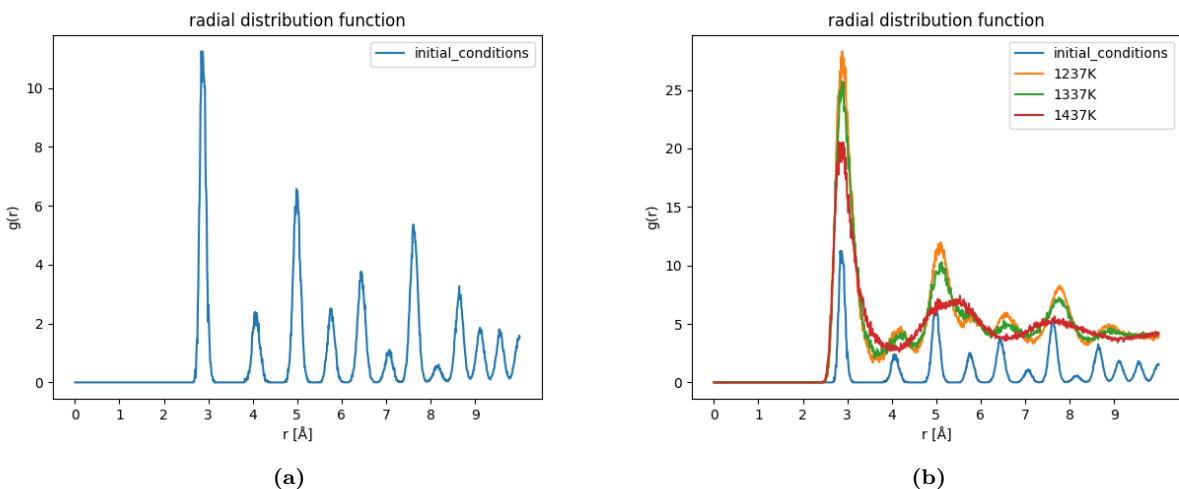
In the provided examples, we have NVT equilibrations with an initial minimization. In these simulations, we aim to study the behavior of the system when fixing the number of particles, volume, and temperature. The examples provided are at  $300K$  and  $1500K$ , and the behavior is simulated for  $1ns$ . When we observe the simulation at  $300K$ , we see that the gold atoms vibrate around their equilibrium positions, maintaining the initial structure of the gold nanoparticle. In contrast, when we observe the simulation at  $1500K$ , we see how the atoms no longer vibrate around the equilibrium positions proper to the nanoparticle but rather disordered and begin to vibrate and move through space. What we are observing here is the difference between atomic behavior in a solid and a liquid.

As with the examples, we could observe the difference in behavior between a solid and a liquid; I found it interesting to study the behavior of the nanoparticle at temperatures close to the gold melting point, so I made a simulation at this temperature ( $1337K$ ) and two more at 100 degrees higher and 100 degrees lower to see if any very sudden changes are perceived or if the changes are more gradual. To do this study, we will focus on studying the radial distribution function and see how the system's temperature, kinetic energy, and potential energy evolve.

### 2.a Study of the Radial Distribution Function

The radial distribution function tells us the number of atoms that we can find at a certain distance from an atom. This function in periodic solids should have periodic peaks at certain distances and be zero outside these distances, and as we increase the temperature, these peaks should gain width because each time we could find atoms more displaced from their equilibrium distances.

When analyzing this function for the 4 cases (Figure 2), we find that for the temperatures where we should find gold in a solid state, we have the peaks at the same distances and without major changes between  $1237K$  and  $1337K$ . However, for the simulation at  $1437K$ , we find that the peaks no longer correspond to the previous ones; in fact, where we had some peaks before, we now find valleys, for example, the peaks at  $4 \text{ \AA}$  and  $6.5\text{\AA}$ . This change in trend clearly indicates how the change from solid to liquid has immediate effects on this function because the change in the function at  $1237K$  and  $1337K$  is very small compared to the change between  $1337K$  and  $1437K$ .

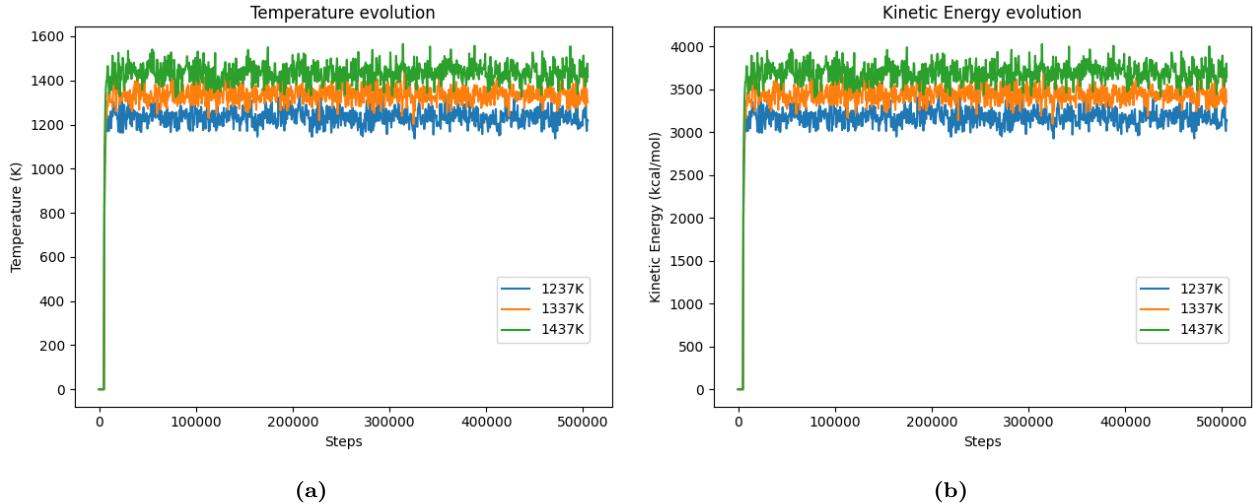


**Figure 2:** **a**, Radial distribution function for the nanoparticle in the initial conditions. **b**, Overlay of the radial distribution functions of the three simulations and the initial nanoparticle.

## 2.b Study of the Evolution of Temperature, Kinetic Energy, and Potential Energy

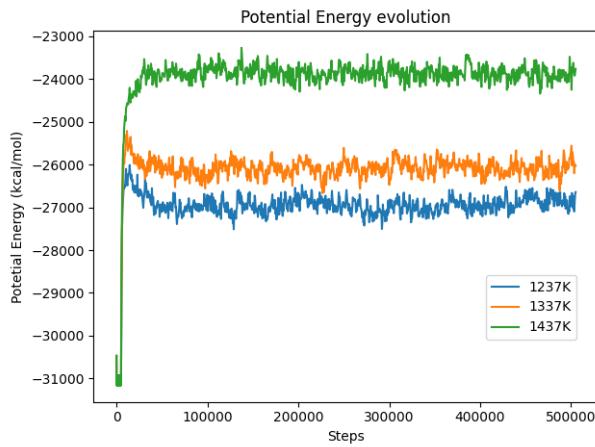
With the study of the evolution of these three magnitudes, we hope to see if we observe any changes in how they evolve depending on the structure, since we observed in the previous section how it changes appreciably as we increase the temperature from  $1337K$ .

With the evolution of temperature and kinetic energy, as we can see in Figure 6, we do not observe any appreciable change, as these magnitudes depend mainly on the temperature. We can see how the temperature and kinetic energy quickly reach their expected values, and there is no change in trend regarding what these values are.



**Figure 3:** a, Temperature evolution. b, Evolution of kinetic energy.

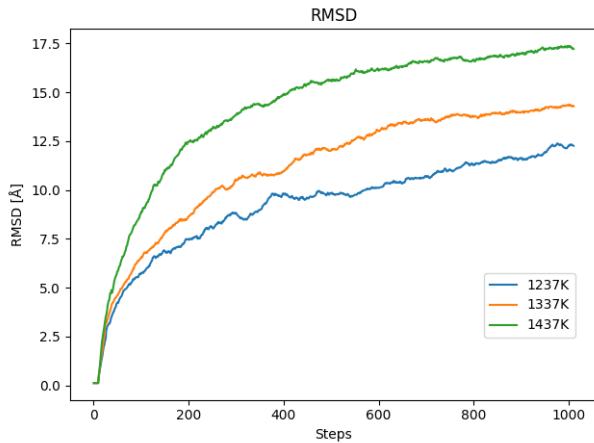
On the other hand, when we get to the potential energy, we do find a change in how this magnitude evolves (Figure 4). We see how the difference in potential energy at  $1437K$  is clearly higher than what it should be if this magnitude depended on the temperature, as the change between  $1237K$  and  $1337K$  is small compared to the change between  $1337K$  and  $1437K$ . This change is due to the fact that while kinetic energy mainly depends on the thermal energy available for the system's atoms, the potential energy of a system of atoms is a very complex magnitude that depends on how the atoms interact with each other, so when changing the phase of our system, we notice a greater change in this magnitude, reflecting the change in the properties of the system.



**Figure 4:** Evolution of the system's potential energy.

## 2.c Study of Atomic Mobility

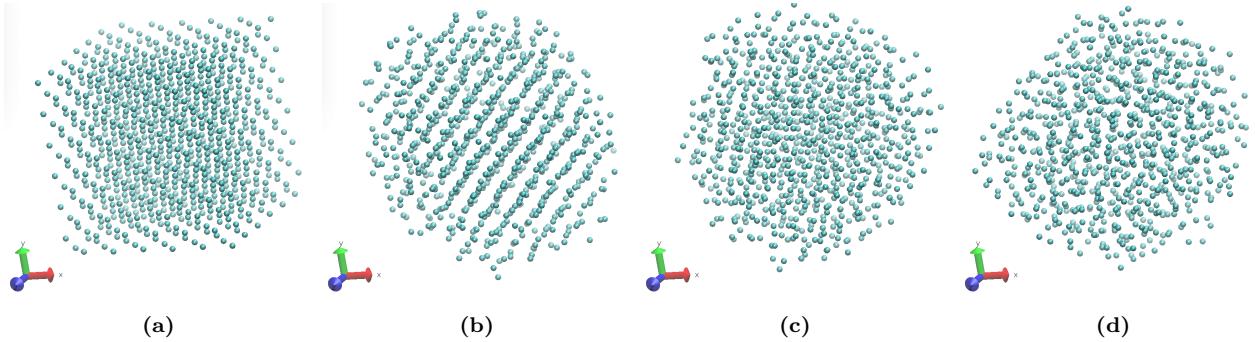
Another study that we can do and is interesting is to verify if when changing phases we find more atomic mobility than simply increasing the temperature. To study this, we can use the “RMSD trajectory” tool incorporated into VMD. This tool gives us information about the average distance that atoms can move from their initial position. When applying this tool to the three simulations, we obtain what we can see in Figure 5. In the figure, we can see how the deviation of the atoms is greater



**Figure 5:** RMDS of the three simulations.

when the temperature is higher, which makes sense. What surprised me when doing this study is how little the atomic mobility increases when changing to the liquid phase, since, although we do notice that the increase between 1337K and 1437K is greater than the increase between 1237K and 1337K, this difference is practically imperceptible, while the change that the structure undergoes is very large.

This surprised me quite a bit, so I decided to compare how the structure was initially with how it was at the end of each simulation; when doing this, I discovered that between the simulations at 1337K and 1437K, there was also not much difference, as we can conclude with the RMSD trajectory study. I think this is because when doing a simulation where the volume is fixed, the atoms cannot disperse as much as they would in a larger volume, and therefore, the maximum distances they can find are smaller. Nevertheless, the big difference between these two simulations is only noticeable when looking at the movie, where much more movement is appreciated in the simulation at a higher temperature.



**Figure 6:** Final structure in initial conditions, at 1237K, at 1337K, and at 1437K respectively.

## References

- [1] “Repositori github.” [https://github.com/DaniBedmar/Lab11\\_MD\\_analysis](https://github.com/DaniBedmar/Lab11_MD_analysis).