

# Simulation of copper nanocluster crystallization

## Computational Nanoscience

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### Abstract

The crystallization of melted copper spheres was studied with 602, 1504 and 3924 atoms. An identical simulation was performed also for a isocahedron Cu sphere with magic number 147. The study was performed with molecular dynamics simulations. The crystallization event was observed from potential and kinetic energies as function of time, temperature as function of time and from caloric curves. The crystallization times were observed and obtained with these methods. In order to be able to predict the crystallization time, a logarithmic function was fitted to the crystallization time data. The crystal structures of the nanoclusters were analyzed with Ovito.

## 1 Introduction

The phase transition is a very widely studied topic within materials science and it has been studied for very long time. It is not only a interesting topic for materials scientists, but also in many other fields, like meteorology. Probably the most studied topic within meteorology today is the global warming. Cluster formation and phase transition play a huge role in it. The impurities and small particles in the atmosphere works as clustering centers for waster droplets [9]. This then affects the cloud formation and thus rain formation and atmospheric radiation [12, 2, 18].

So understanding how the particles form in the atmosphere is obviously important. Not only how the particles are formed, but also how different kind of particles affect the physics of atmosphere. In this study the effect of cluster size is studied to observe what kind of crystal structures is formed to the solidified copper clusters.

## 2 Methods

This study is performed with molecular dynamic simulations using LAMMPS [8]. The analysis of the molecular dynamics simulation results is done with Ovito and python [11, 15]. Three different sized Cu clusters were simulated and one Cu icosahedron with magic number 147.

## 2.1 Simulation

The simulation was performed in argon atmosphere with pressure of 20 bar. The initial condition consisted of Cu sphere with FCC lattice and the Ar atmosphere with FCC lattice. The Cu cluster was melted in 3000 K with nvt ensemble while keeping the Ar atmosphere in 50 K with nvt ensemble. Before the melting simulation, a short minimization run was done to remove unnatural tension from the system. The Cu sphere was heated long enough to make sure it was melted.

After the melting a minimization run was done to stabilize the system. The Ar atmosphere was kept in 50 K with ntv ensemble. The Cu cluster was set to nve ensemble and it was cooled by the Ar atmosphere for 10 ns. In the end a short minimizing run was performed to remove the thermal noise from the system.

During the simulation, Ar pressure was computed from the stress vectors of Ar atoms. Also Cu atoms and Ar atoms temperatures were computed during the simulation [8]. For Cu-Cu interactions EAM potential model was used. EAM potential for Cu atoms has been well established and it has been proven working well [3, 17]. Interactions between Cu-Ar and Ar-Ar was modeled with ZBL potential. The potential was purely repulsive to model realistic interactions with noble gases [20].

## 2.2 Estimation Of Ideal Gas Pressure

Task 2 in project 1 was to estimate the Ar gas pressure from ideal gas law. The ideal gas law is

$$pV = nRT, \quad (1)$$

where  $p$  is gas pressure,  $V$  is system volume,  $n$  is the amount of substance,  $R$  is the ideal gas constant and  $T$  is the system temperature. To solve the Ar gas pressure we can divide the equation with volume to calculate the gas pressure.

$$p = \frac{nRT}{V}. \quad (2)$$

## 2.3 Correspondence Of Kinetic Energy And Temperature

The corresponding kinetic energy of certain temperature was calculated in order to see how well the observed temperatures of crystallization events correspond to kinetic energies of the same events. The corresponding kinetic energy was calculated with the following equation

$$K_e = \frac{\dim}{2} N k_b T, \quad (3)$$

where  $N$  is the number of atoms in the group,  $k_b$  is the Boltzmann constant,  $T$  is the temperature and  $\dim$  is the number of dimensions in the system [8].

The number of dimensions in this simulation is 3 as the system is simulated in 3-dimensional space.

## 2.4 Crystallization Time

A logarithmic function was fitted to the data obtained from crystallization times as function of cluster size. The following logarithmic function was used

$$f(x) = a \times \log(bx) + c. \quad (4)$$

For the fitting a *curve fitting* method of *scipy.optimize* library of python3 was used to fit the function to the data [1, 16].

# 3 Implementation

## 3.1 LAMMPS Simulation

The simulation consist two types of atoms; copper (Cu) and argon (Ar). The atomic unit mass used for the are Cu = 63.55u and Ar = 39.95. The initial simulation set-up is performed by creating first a copper sphere with FCC structure with lattice spacing of 3.61. Three different sized Cu clusters were made with radius of 3.3 Å, 4.5 Å and 6.15 Å. They do correspond Cu clusters with 602, 1504 and 3924 atoms. The icosahedron of 147 atoms was obtained from exercise set 09 materials. No energy minimization of any kind was yet performed for the produced Cu clusters. Every simulation had a constant number of 3287 Ar atoms.

The actual simulation was performed with metal units, atom style atomic and periodic boundaries to all three dimensions [8]. The simulation box is created by reading the Cu sphere data file. It creates a simulation box with edge length of 120 Å. Then a FCC lattice is created with lattice spacing of 12.5. The Ar atmosphere is then created by creating a empty sphere shaped region to the middle of the simulation box with radius of 2.0 Å. The rest of the simulation box is then filled with Ar atoms. This way an Ar atmosphere of about 20 bar is created. The much larger pressure, than regular atmospheric pressure, is set to obtain shorter simulation times [4]. As potential model for Cu-Cu interactions a EAM potential was used. Cu-Ar and Ar-Ar interactions was modeled with ZBL potential model to obtain purely repulsive interactions.

The simulation was performed by using time steps of 0.001 ps. A short minimization run was performed in the beginning of the simulation with LAMMPS *minimize* command for 10 000 steps. Then a initial velocity of 3000 K was applied for Cu atoms and 50 K was applied for Ar atoms. The Cu cluster was then melted in 3000 K in nvt ensemble while keeping the Ar atmosphere in 50 K with nvt ensemble. This was performed for 20 000 steps to make sure the Cu sphere has molten.

After the Cu sphere is molted, a short minimization run of 10 000 steps was performed. This system state is then writed to *molted.data* to be able to check

that the Cu sphere has really been molted. After the system initialization the Cu cluster is set to nve ensemble while floating in the Ar atmosphere which is still fixed to 50K with nvt ensemble. The Cu cluster is now cooled by the interactions with the Ar atmosphere and the atmosphere removes the extra heat with Nosé-Hoover thermostat [6, 7, 13, 10]. The system was run 10 000 000 steps to obtain a simulation time of 10 ns. After these steps a last minimization run was performed to remove the thermal noise. The resulting system was saved to a data file.

During the simulation, the following properties were calculated and saved to \*.log file or \*.dump file.

- Argon Gas Pressure
- Potential Energy / Atom
- Kinetic Energy / Atom
- Orient Order / Atom
- Temperature Of Cu Atoms
- Temperature Of Ar Atoms
- Step
- System Temperature
- Total Energy
- System Pressure
- System Volume
- Time

In order to prevent the Cu cluster to move through the simulation box a LAMMPS command was fixed in order to do this.

```
fix           CENTFIX atoms_Cu recenter INIT INIT INIT shift all
```

This command was not unfixed through the simulation to keep it working. This command was set before any `run` command. The `minimize` commands used `min_style cg` for the minimization.

### 3.2 Data Analysis With Python

The .log files were analysed with python3 with a jupyter notebook. To be able to read the \*.log files straight to pythons pandas data frames, a bit preprocessing was performed. The log files were preprocessed with a `gawk` command.

```
gawk '$1=="ec" {print}' *_cu_sphere*.log > *_cu_sphere*.csv
```

The command searches from column 1 lines which starts with string `ec`. This is added to the log files with command

```
thermo_style    custom step temp pe etotal press vol time v_press_Ar c_temp_Cu c_temp
thermo_modify   line one flush yes format 1 "ec %8lu" format float "%20.10g"
```

The asterisks correspond to simulation size (small, medium, large) and simulation number (1,2,3,4). The resulted \*.csv file can now be read straight to pandas data frame. The plotting and data analysis of the files has been done with jupyter notebook `plotting.ipynb` and it can be accessed immediately, but it cannot be run without the files. All the plots can be seen if it is not tried to run.

### 3.3 Structure Analysis With Ovito

The structure analysis was done with Ovito [11]. To obtain the same structure analysing situation as in this study, the following commands were used in this order for files `*_cu_sphere*_result.data`. The asterisks corresponds again to simulation size and number.

- Add modification "Select Type"
- Select then "Type 2"
- Add modification "Delete Selected"
- Add modification "Polyhedral Template Matching"
- Add modification "Select Type"
- Select then type "Other"
- Delete Selected

The Polyhedral Template Matching can find different type of lattice structures from the system [5].

## 4 Results

The simulations worked quite smoothly, but I didn't got the command `recenter` working until simulation sequence 4. In those simulations 4, the temperatures for Cu atoms and Ar atoms was also calculated so they are the simulations I will be focusing in here. Some of the simulations ended up having the cluster at the edge of the simulation box's side so the cluster was splitted in half. This doesn't though affect the results, but whole clusters are easier to visualize.

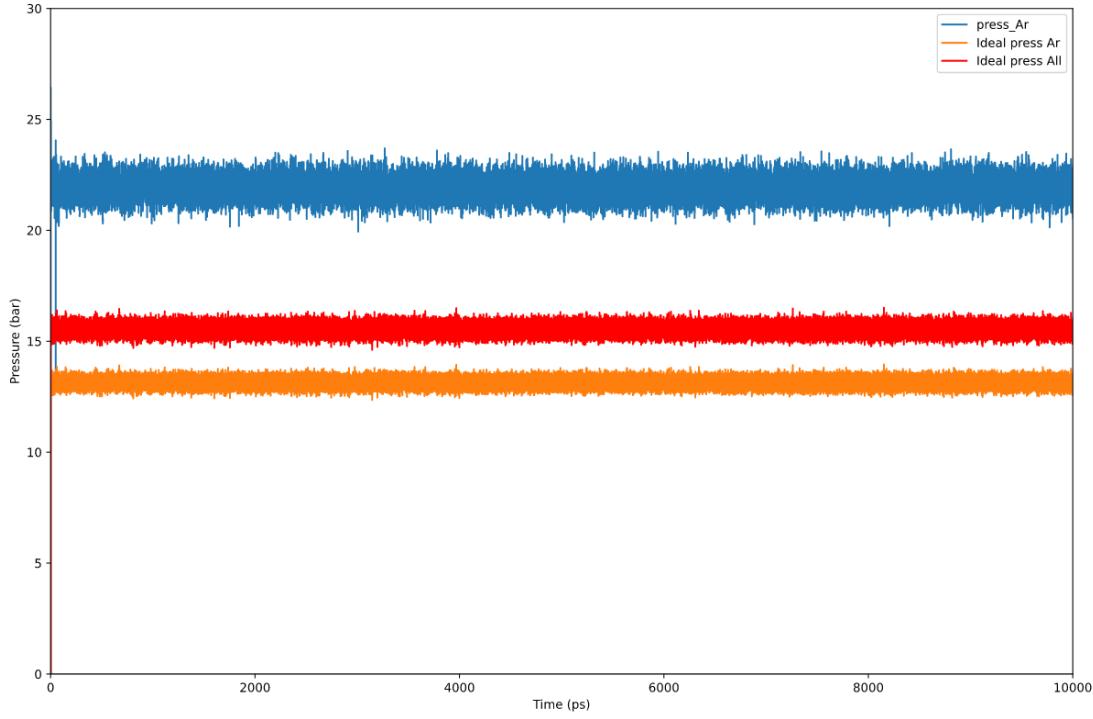


Figure 1: The gas pressures presented as function of time. The blue one corresponds to Ar pressure obtained from the \*.log file and the Ideal press Ar and All are calculated with the ideal gas equation. First one having only the Ar atoms and second one including both Ar and Cu atoms. This data obtained form simulation Small4

#### 4.1 Estimating Argon Gas Pressure From The Ideal Gas Law

The first task after setting the simulation up was to estimate the Ar gas pressure from ideal gas law and compare it to values gotten from the simulations. With the ideal gas law (2) we can estimate the Ar gas to have pressure of 13.13 bar at temperature of 50 K. This is lower than the value of Ar pressure calculated to the log file. From figure 1 we can see that it doesn't even change as function of time.

The pressure of ideal gas seems to be lower for Ar gas calculated from ideal gas law. Adding the Cu atoms to the calculation doesn't explain the difference. Even though the ideal gas pressure is quite close to the one obtained from log file, there is something in the simulations that increases the Ar gas pressure. It can't be explained by the hot Cu cluster because the pressure it not decreasing. The same plot was made with different cluster sizes to see if there is an effect in the cluster size. The results can be seen in figure 2.

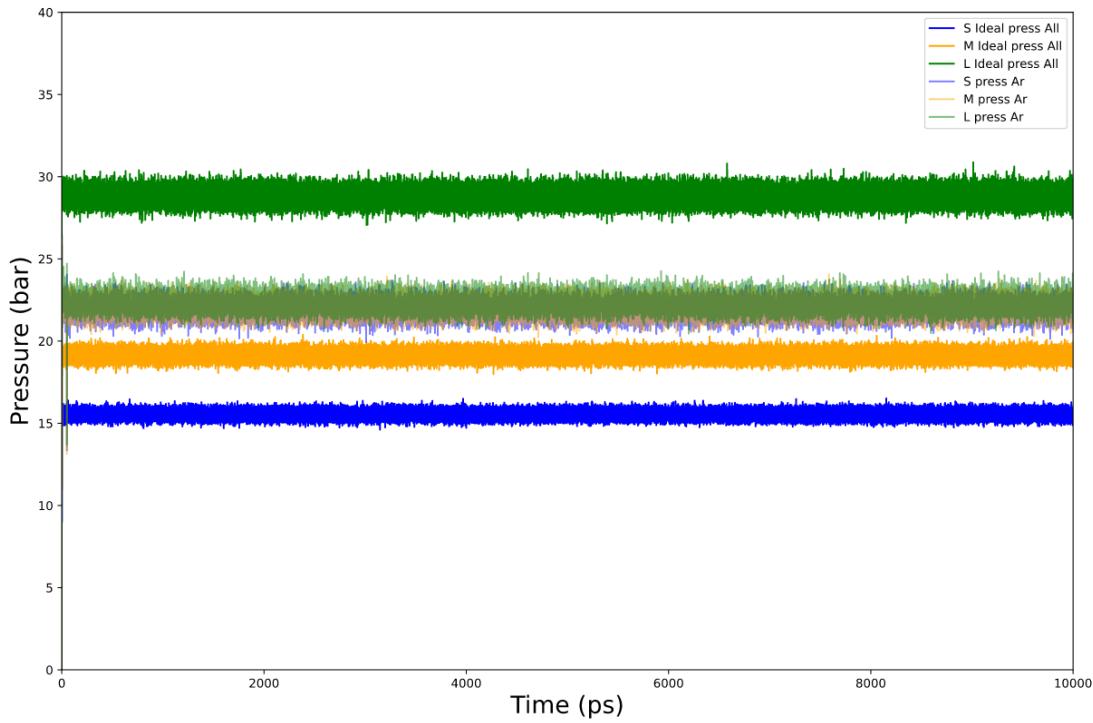


Figure 2: The ideal gas pressure values including also the Cu atoms in the simulation. The press Ar line with three line on top of each other is the Ar pressure data from the \*.log files.

The letters S, M and L corresponds to Small, Medium and Large simulations. So figure 2 confirms now that the Cu cluster doesn't have effect to the ideal gas pressure of Ar atmosphere. It is clearly seen that with more atoms, the pressure is greater, but the Ar pressure obtained from log files, still stays the same. From figure 2 and the previous figure 1 we can though see that the ideal gas pressure in all cases is still smaller than in the values from log files. The gas pressure of Ar calculated to log files, is calculated by the stress vectors of Ar atoms and it is probably more accurate that the ideal gas law pressure. The interaction potential used for Ar atoms is only repulsive so it is quite realistic for noble gases like Ar. This is probably more accurate way to calculate the gas pressure than the ideal gas law. Both ways of calculating the pressure though confirms that the simulation has been done in constant Ar atmosphere pressure.

#### 4.2 Observing Crystallization Of Copper Nanocluster

The second task was to explain how the crystallization (phase transition) was observed. Few methods were mentioned in the article by Valkealahti et al; "The

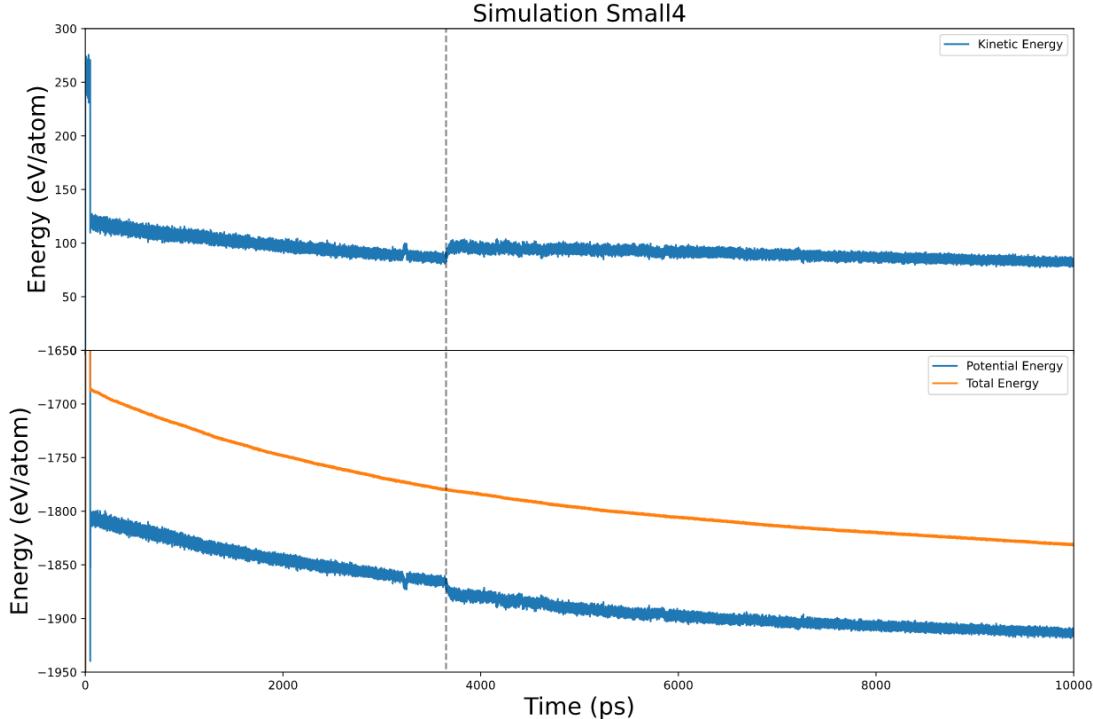


Figure 3: The crystallization time can be observed from the little steps from the kinetic and potential energy curves. The potential energy transfers to kinetic energy during the crystallization and thus the steps. The total energy is the sum of kinetic and potential energy and thus a step is not observed in it [14]. The total energy is a constant in small enough timescales, but as the system energy decreases, the total energy decreases also.

crystallization of copper clusters was analysed by means of total, potential, and kinetic energies as functions of time and temperature, root mean square displacements of atoms, and snapshots of clusters.” [14]. So to observe crystallization event we can use the methods described above which has been used by Valkealahti et al. In this study caloric curves and energies as function of time was used to observe the crystallization times.

We can first use the energies of atoms as function of time. The total energy should only decrease through the whole simulation and be constant in short intervals as it is the sum of kinetic and potential energy. The crystallization can be though be observed from the transition of potential energy to kinetic energy. This is because when the cluster crystallizes, its lattice energy is minimized so the potential energy decreases. This means that the decreased potential energy has to go somewhere and it is transferred to kinetic energy and the atoms kinetic energy rises and thus leads to rising temperature in the cluster [14]. The

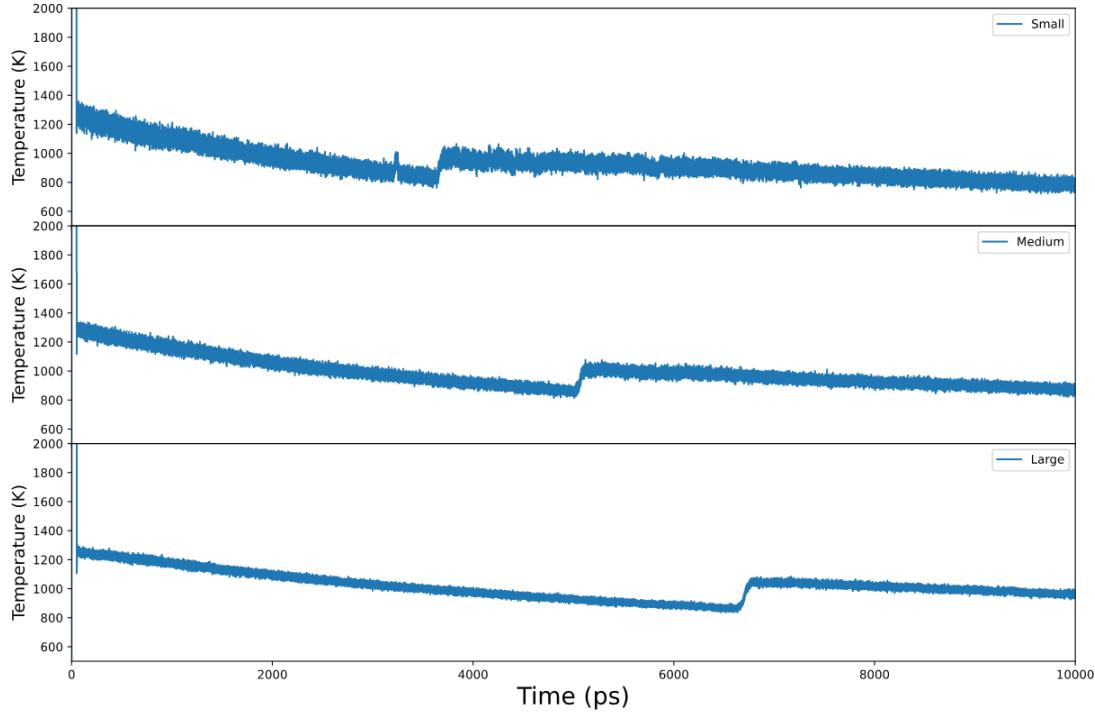


Figure 4: The crystallization event can be observed from the steps. From the top figure, an attempt to crystallize can be seen a bit before the actual crystallization event. The temperature during the attempt was probably still too high to be successful and a bit more cooling was still needed.

crystallization event was first tried to observe from small cluster (Sim4) in figure 3.

The crystallization event can be seen quite clearly from the figure 3. The dashed line is added to help to notice the step. One thing to notice is that the used energies are the sum of all atoms in the system. So these energies include also the Ar atoms energies. This doesn't hinder though because the kinetic energy of Cu atoms is so much larger so that the effect of can still be seen, as observed in figure 3. To have a more clear step to observe, the energies of Cu atoms should have been calculated separately. But as mentioned before, when the potential energy transfers to kinetic energy, the cluster temperature rises. This way we can observe the effect of cluster size in crystallization time. Luckily the temperatures for Ar and Cu atoms separately were calculated. The results of this can be seen in figure 4.

With smaller cluster the temperature fluctuates more and it can be seen as a wider line. Also the bigger the cluster is, the longer it takes for it to cool and it can be seen from the steps the lines make, attends to be later with larger

cluster size.

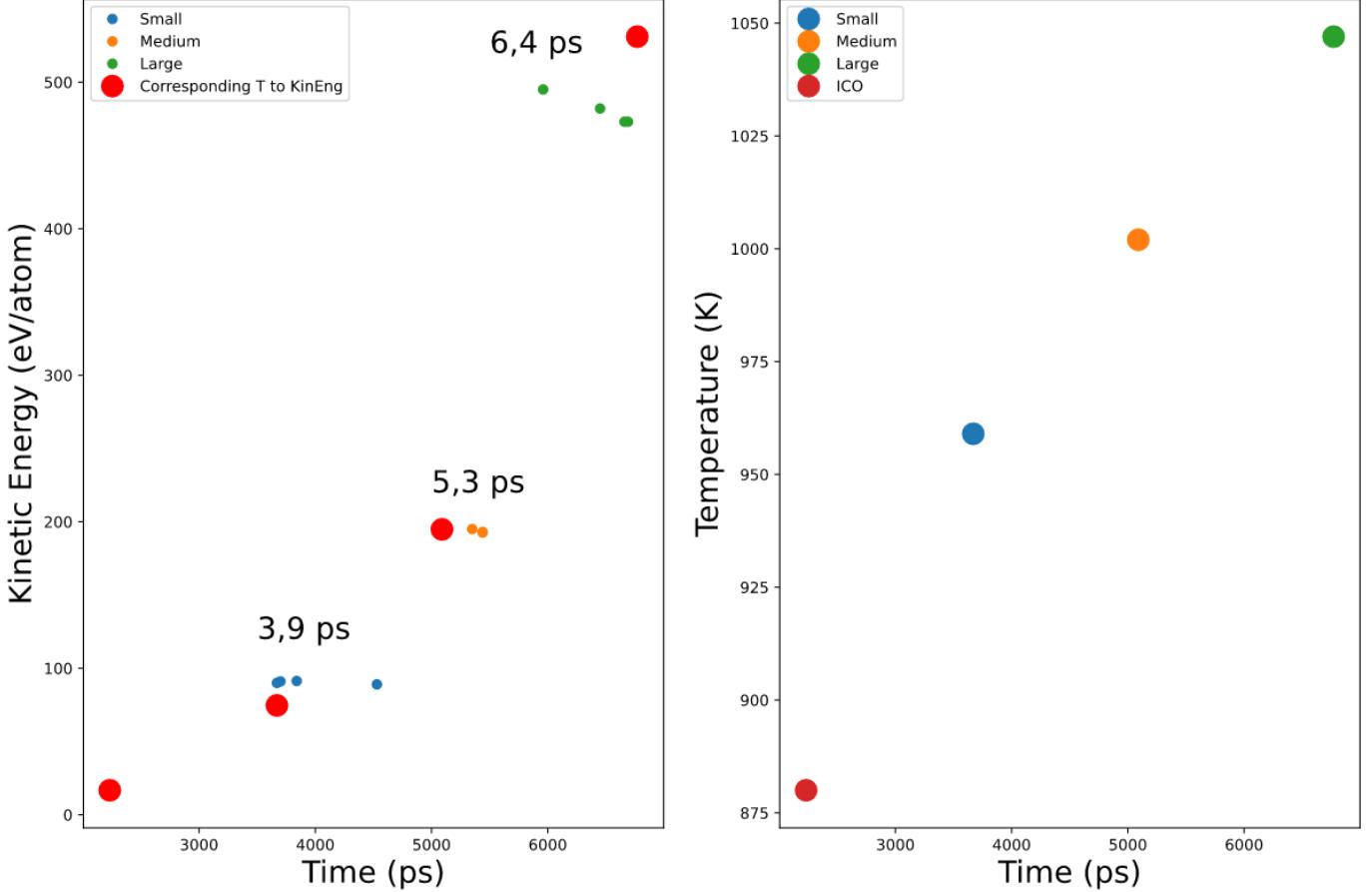


Figure 5: The numbers on the left figure correspond to the mean crystallization time of each cluster size. The red dots are the corresponding values from the right figure. It can be seen that they align quite well with the other data points even though the kinetic energies are calculated from the sum of all atoms in the system.

Does the crystallization time fluctuate or how stable the time is? The cluster temperatures was measured only in simulations 4, but we can measure the time from the kinetic energy for each simulation and these times can be observed from the figure 12 in the appendix. It is quite hard to see the exact crystallization points from the figure, but the numbers I got by hand approximating from the figure are presented in 6 and table 1 which can be found from the appendix.

So initially I tried to calculate the crystallization temperature from the kinetic energy, but because the kinetic energy is the mean of all particles kinetic

energy, I couldn't calculate the temperatures for Cu cluster. The corresponding kinetic energies from the fourth simulations are presented as red dots on the figure 6 on left.

The corresponding kinetic energy was calculated from kinetic energy function. The corresponding temperature for particles are calculated from the same function 3. The crystallization temperature seems to rise as function of cluster size. This is logical and follows the observations of Cu cluster melting temperatures from exercise set 09. The crystallization temperatures were about the same as in similar study from Wu et al with same sized Cu atoms [17]. I didn't find mentions about the system pressure in Wu et al paper. In my simulations the Ar atmosphere was set to pressure of about 20 bar. This leads to higher melting and solidification temperature, so the temperature values here might differ from exercise 09 [19]. In the study of Wu et al, the cooling was done with speed of  $15 \times 10^{12} \text{ K s}^{-1}$  and the fast cooling speed was  $30 \times 10^{12} \text{ K s}^{-1}$ , but in our simulation the hot and melted 3000 K Cu sphere was dropped instantly to an argon atmosphere heat bath of 50K in high pressure so it was cooled very fast to around 1300 K and from there it was cooled much slower. The plot can be found from appendix figure 13.

The crystallization times though could be obtained from the plots and the means for each cluster size crystallization temperature is shown if figure 6 on left side. Now we can see how does the crystallization time behave as function of cluster size.

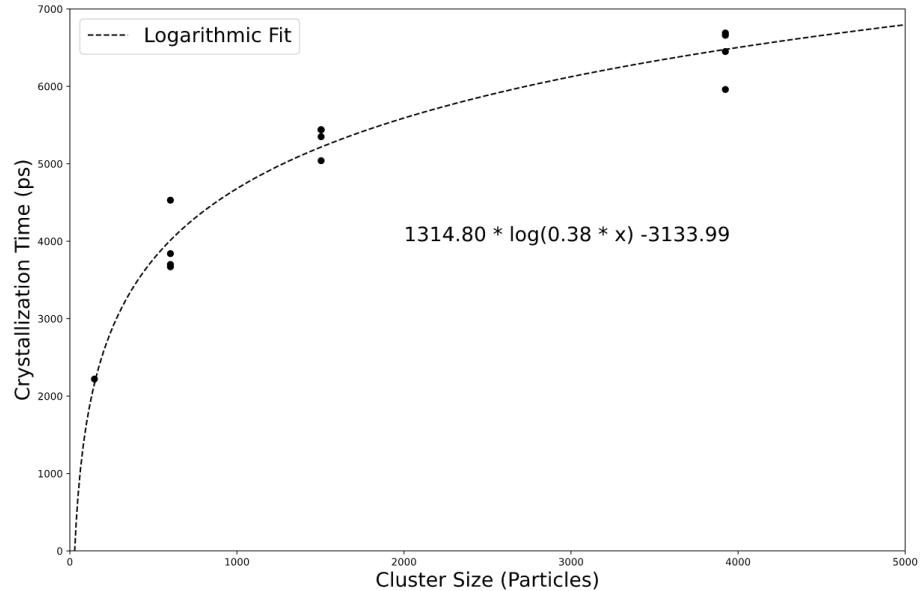


Figure 6: Crystallization time as function of cluster size.

So here we can see that it's behavior seems logarithmic and a logarithmic

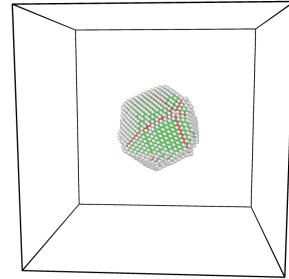
function does sit quite well in the data points. The one data point on the left is the data point of the 147 icosahedron and it probably has a huge impact to the beginning part behavior of the logarithmic function. The logarithmic function:

$$1314.80 \times \log(0.38x) - 3133.99 \quad (5)$$

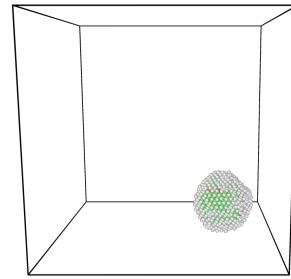
With this equation we can predict the crystallization times, if the cluster size is known.

### 4.3 Structural Characterization With Ovito

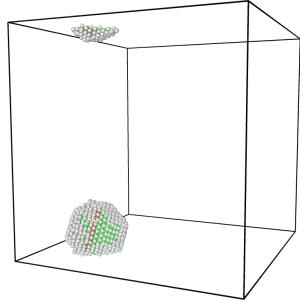
As mentioned in the beginning of this chapter, I got the `recenter` command working only in the simulation sequence 4, so some of the earlier simulations might have ended so that the clusters were splitted because of the periodic boundary conditions or just ended otherwise being shifted from the center.



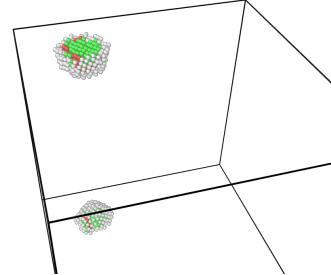
(a) Large Cu cluster.



(b) Medium Cu cluster not sliced, but being a little offset from the center.



(c) Medium Cu cluster sliced.



(d) Small Cu cluster sliced.

Figure 7: End results from different simulations. Only 7a had `recenter` command working properly.

Because the sliced clusters are harder to visually analyze, only the cluster from simulation sequence 4 are analyzed visually. In those clusters also the thermal radiation noise has been removed by minimization, so they are also that

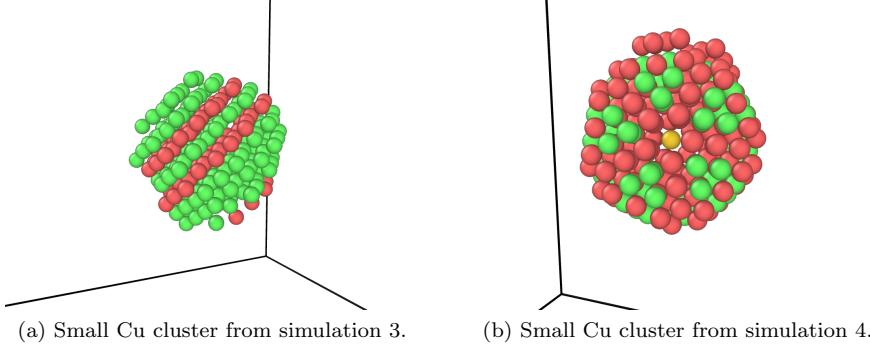


Figure 8: Cluster in figure 8a has three FCC grains separated by HCP layers. Icosahedral shape can be observed from figure 8b.

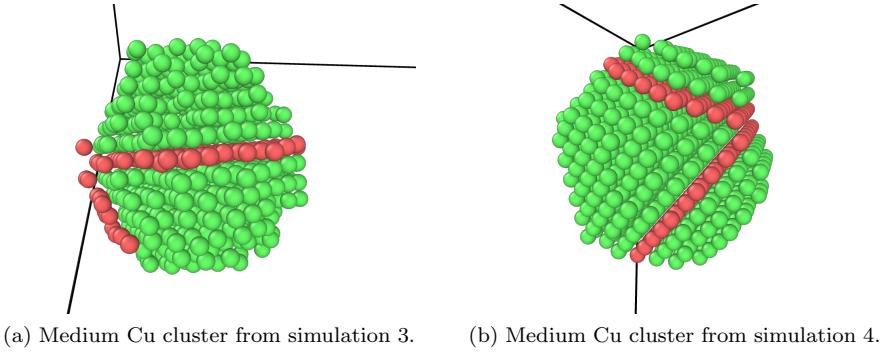


Figure 9: Medium sized clusters is separated to FCC grains separated by HCP layer and no icosahedral structures can be found.

way better to analyze. In the figures white particles corresponds to OTHER type of atoms, green ones to FCC, red ones to HCP and the few yellow ones to ICO.

As seen from the figure 8 the effect of minimizing can be seen clearly. As claimed in the paper of Valkealahti et al, the Cu clusters below 2000 atoms should crystallize to icosahedral structures as it is the most stable structure for them [14]. In 8a the FCC grains are separated by HCP layers and the most stable structure hasn't been yet achieved because of the thermal energy affecting the cluster. In the other hand, in figure 8b the icosahedral structure can be seen very clearly. The yellow atom in the middle of the cluster is the symmetry point of icosahedron. When the atom number approaches 2000 atoms, the icosahedral structure can't be seen at least in medium sized cluster.

Valkealahti et al mentions that larger clusters tend to crystallize to twinned FCC structures with typically three to five FCC grains and with these medium sized clusters it is verified [14]. The interesting part is with the large cluster sizes, because 3924 atoms is already twice as much atoms than the margin of

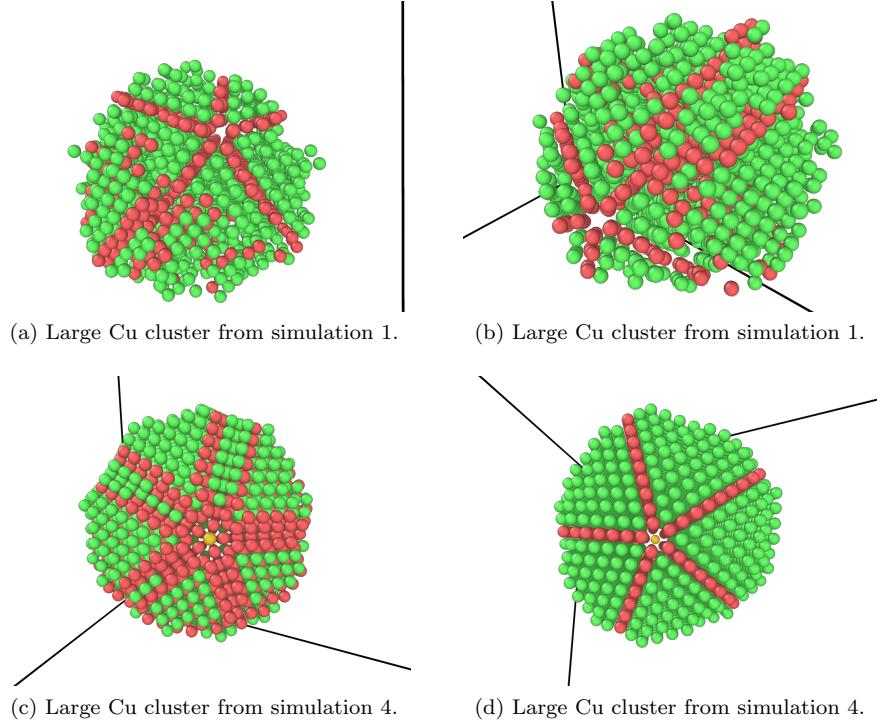


Figure 10: Large Cu clusters from simulations sequences 1 and 4. Cluster from simulation 1 appeared two start crystallize to two directions.

2000 atoms.

Interestingly enough, even these large cluster with atoms closer to 4000 tended to crystallize to FCC lattice grain separated by HCP layers. In figure 10a and 10b the cluster tends to crystallize from two view points and similar star shaped structures can be observed from two different points. With small minimization run, the other crystallization site might have vanished. But the curiosity here is that in the simulation 4 of the large Cu sphere, we can observe some icosahedral features. The yellow particle at the tip of the cluster in figures 10c and 10d is the symmetry point of icosahedron. Even though there is no icosaheron formed, but some symmetry of icosaherdon is clearly seen in the cluster. The star shape can be seen more clearly from figure 14 in the appendix.

#### 4.3.1 Icosahedron With Magic Number 147

As mentioned by Valkealahti et al the Cu clusters with less than 2000 atoms tends to crystallize to icosahedral structure. They also mentioned that the small Cu clusters with magic number of atoms like 13, 55 and 147, crystallizes directly to a icosahedron, so I had to test it [14].

From figure 11 we can clearly see that this is verified. The simulation was

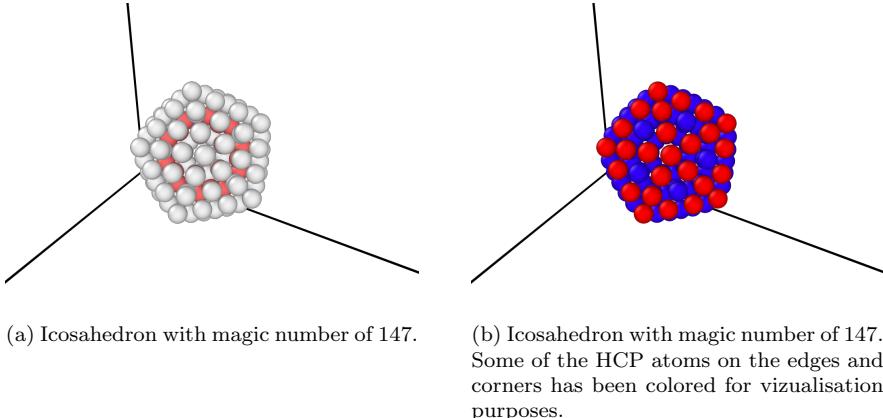


Figure 11: Icosahedron-147

done in same conditions as the other clusters and a small minimization run was done in the end of the simulation. The starting shape of the simulation sphere was a 147-icosahedron obtained from exercise set 09. From figure 11 we can clearly observe that it has formed a perfect icosahedron.

## 5 Conclusions

With well established potential models and tools, no new physical properties or events were observe in this study. Using LAMMPS for this study was quite obvious, but while reading the papers related to this study, it just shows how this kind of simulations can be done in multiple ways and all those different simulations could be performed with LAMMPS. So it is a quite powerful tool when used properly.

The results from the simulations were analyzed with python and Ovito. Python was used to observe the crystallization (phase transition) times for the clusters. The crystallization time was obtained from the energies as function of time, temperatures as function of time and the caloric curves. The crystallization times in this particular environment seemed to have logarithmic properties and a logarithmic function was fitted to the data. The function could be used to predict crystallization times in similar environments.

Structural characterization was analyzed with Ovito. A plot and a table from all simulations structure percentage can be found from the appendix from figure 15 and table 2. The small cluster crystallized to a icosahedral structure and the medium and large sized clusters crystallized to 3-5 FCC grains separated with HCP layers. The results obeys observations and results of Valkealahti et al [14]. Also the icosahedron with magic number of 147 crystallized directly back to icosahedron when cooled enough.

## 6 Acknowledgement

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## 7 Appendix

This is the appendix and it contains figures and tables which were not shown in the report.

	$t$ (ps)	$K_E$ (ev/atom)
S1	3840	91.3
S2	3700	91
S3	4523	89
S4	3670	90
M1	5350	195
M2	5440	193
M3	5440	192.6
M4	5040	196
L1	6450	482
L2	6660	473
L3	5960	495
L4	6690	473

Table 1: Crystallization times and energies of the clusters.

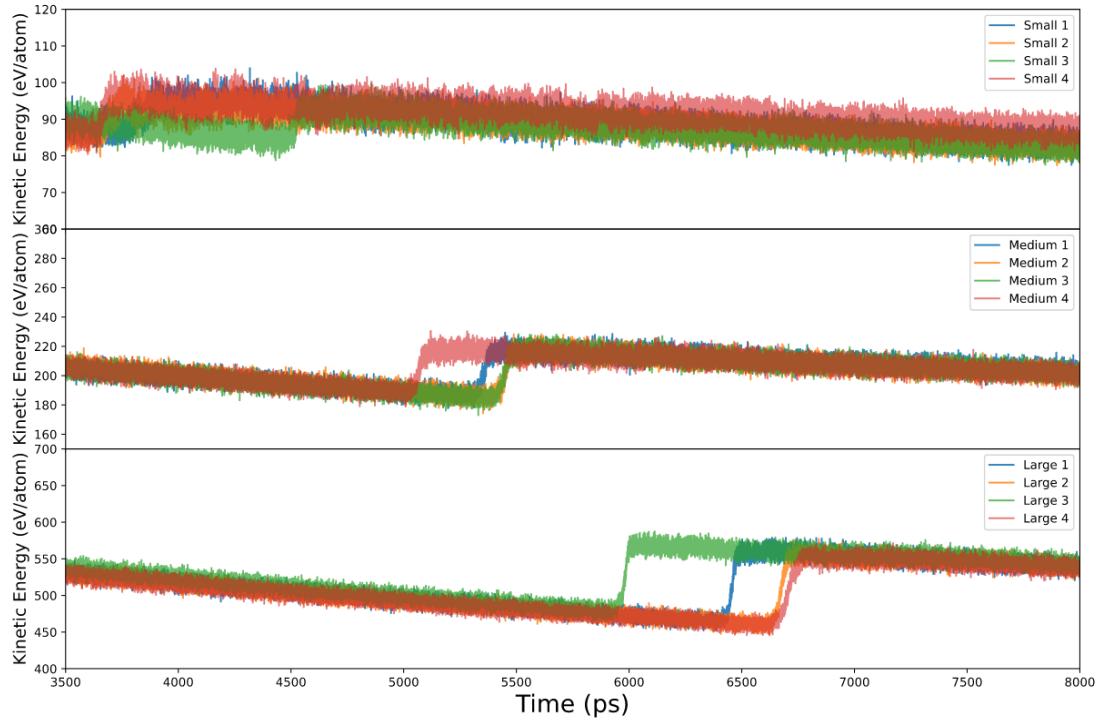


Figure 12: Kinetic energies as function of time to observe the crystallization times of different sized clusters.

	Other (%)	FCC (%)	HCP (%)	ICO (%)
S1	57.4	34.8	7.8	0.0
S2	59.9	38.3	1.8	0.0
S3	54.6	31.3	14.1	0.0
S4	53.9	13.3	32.7	0.2
M1	53.2	40.9	5.8	0.0
M2	53.9	34.5	11.6	0.0
M3	54.8	32.5	12.7	0.0
M4	26.1	53.8	10.0	0.0
L1	57.0	32.3	10.7	0.0
L2	51.7	35.3	13.0	0.0
L3	54.5	31.1	14.4	0.0
L4	28.6	52.3	19.1	0.0
ICO	78.9	0.0	20.4	0.7

Table 2: Structure percentage of each simulation result.

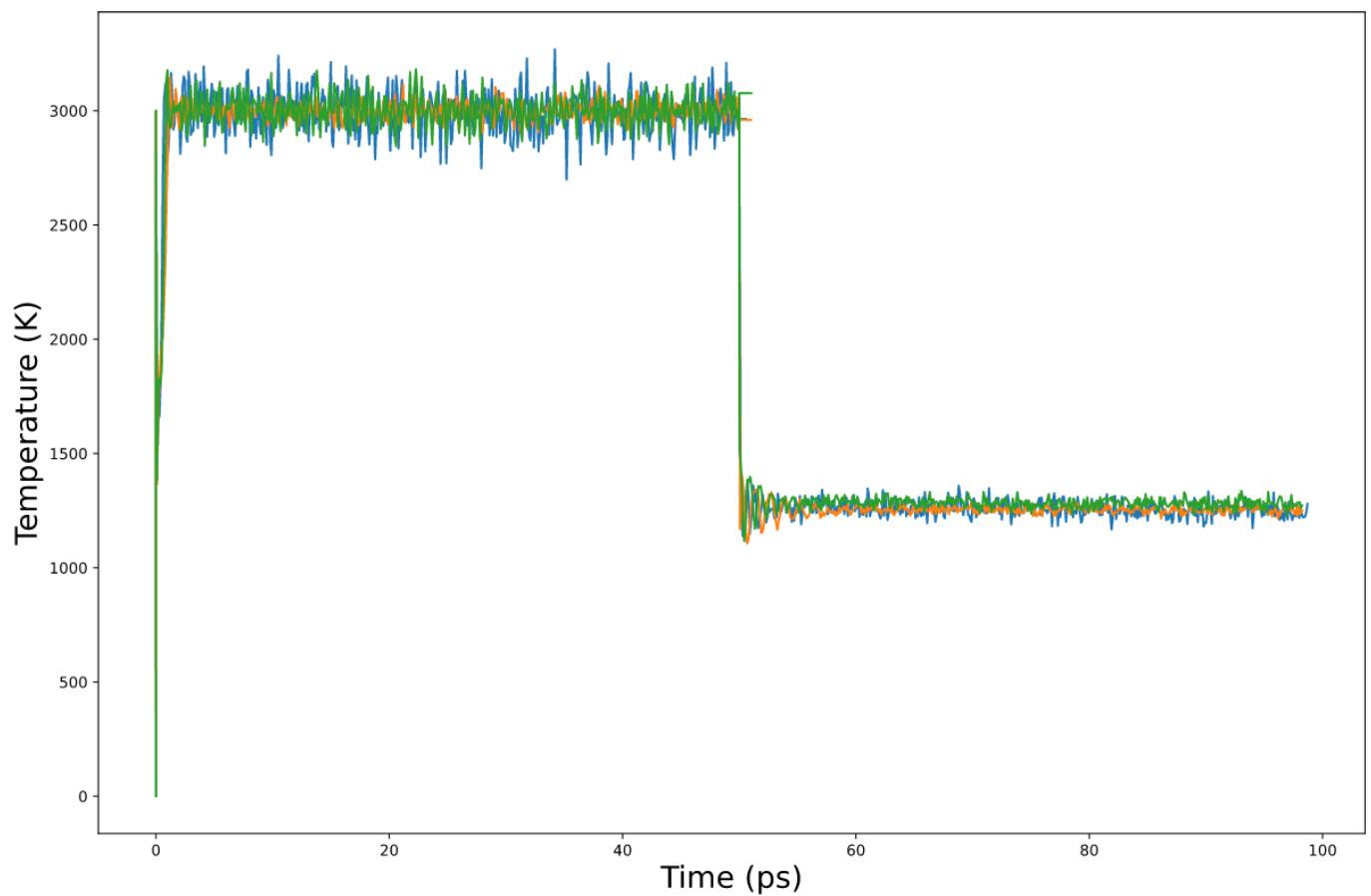


Figure 13: The fast heating and cooling of Cu cluster.

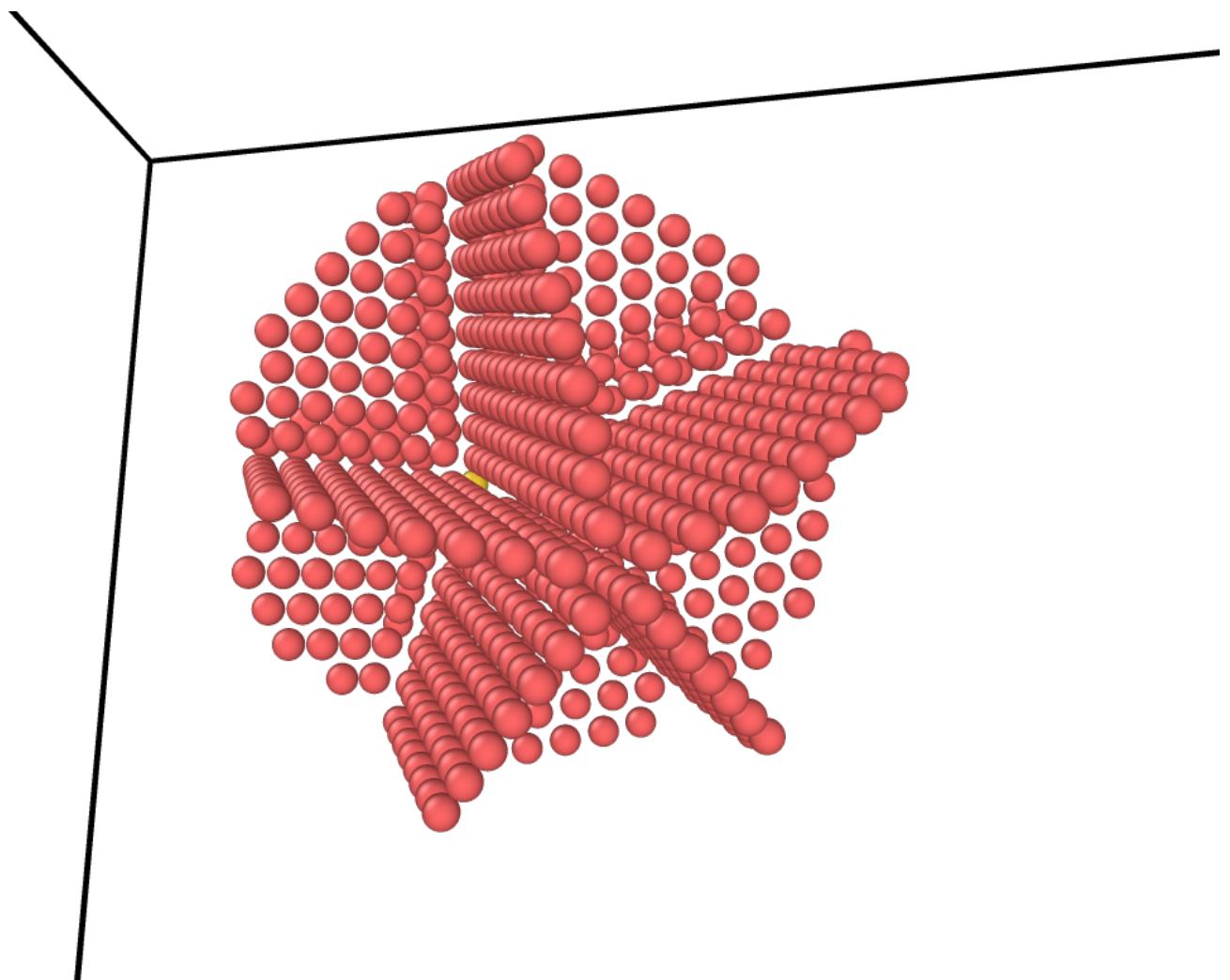


Figure 14: The large Cu cluster from simulation 4 with FCC atoms removed.

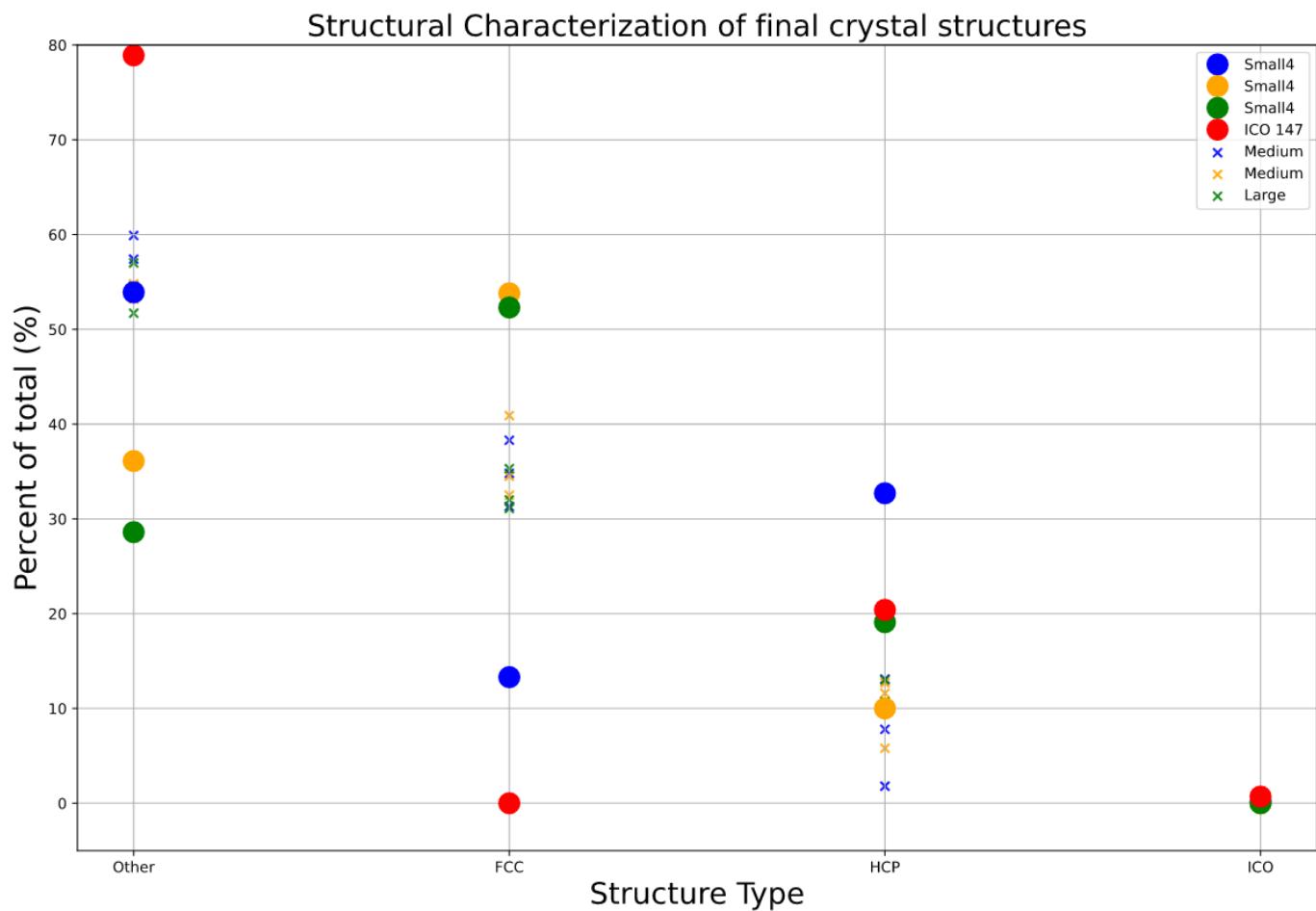


Figure 15: Structure percentages of each simulation. Simulation sequence 4 expressed with larger dots because more accurate results were obtained due to the minimization in the end.

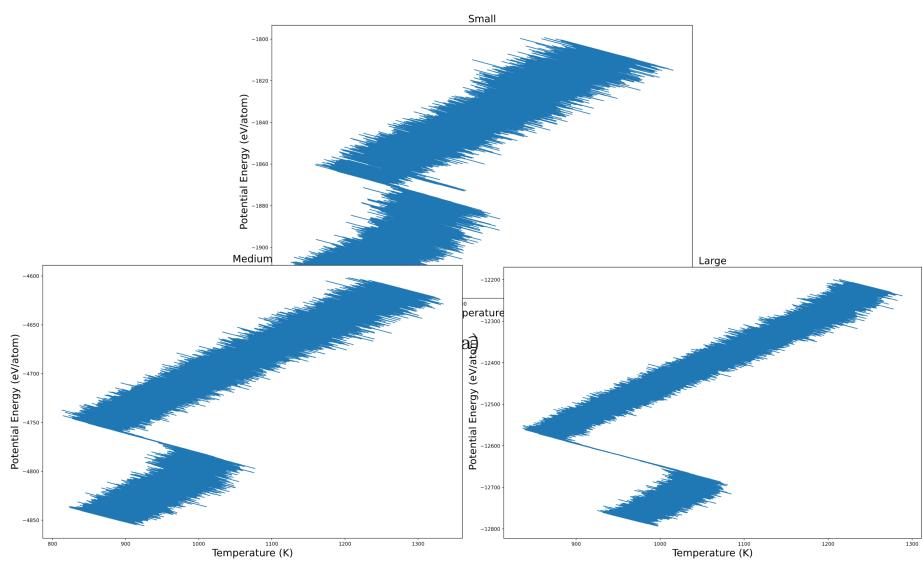


Figure 16: Caloric curves for small, medium and large from simulation sequence 4.