

¹School of Physical Sciences and Nanotechnology, Yachay Tech University,
100119-Urcuqui, Ecuador



²SINanO team, Centre d'Élaboration de Matériaux et d'Etudes Structurales,
31055-Toulouse, France



Controlling Seed Crystallization using LAMMPS

February 16, 2023

Internship Report

Leonel A. Cabrera¹, BSc student.

Supervised by:
Akshay Ammothum², Ph.D.
Julien Lam², Ph.D.

Contents

1 Introduction	3
2 Methods	3
2.1 The Radial Distribution Function	3
2.2 Bond-orientational order parameters	4
3 Simulation Details	5
4 Challenges	6
5 Small systems results	7
5.1 Density = $1175/40 \times 40 = 0.734$	7
5.1.1 Crystal seed of 55 atoms	7
5.1.2 Crystal seed of 109 atoms	8
5.1.3 Crystal seed of 163 atoms	8
5.2 Density = $1100/40 \times 40 = 0.687$	9
5.2.1 Crystal seed of 55 atoms	9
5.2.2 Crystal seed of 109 atoms	9
5.2.3 Crystal seed of 163 atoms	10
5.3 Density = $1025/40 \times 40 = 0.640$	10
5.3.1 Crystal seed of 55 atoms	10
5.3.2 Crystal seed of 109 atoms	11
5.3.3 Crystal seed of 163 atoms	11
5.4 Densities lower than 0.640	12
5.5 Final Analysis: RDF vs Seed Size	12
5.6 Final Analysis: RDF vs Lattice Spacing	13
6 Large Systems Results	15
6.1 Density = $10000/116.72 \times 116.72 = 0.734$	15
6.1.1 Crystal seed of 37 atoms	15
6.1.2 Crystal seed of 55 atoms	15
6.1.3 Crystal seed of 109 atoms	16
6.2 Density = $9359/116.72 \times 116.72 = 0.687$	16
6.2.1 Crystal seed of 37 atoms	17
6.2.2 Crystal seed of 55 atoms	17
6.2.3 Crystal seed of 109 atoms	17
6.3 Looking for crystallization in large systems with a crystal seed of 37 atoms	18
6.4 Final Analysis: RDF vs Seed Size	18
6.5 Final Analysis: RDF vs Lattice spacing	19
7 Conclusions	20

1 Introduction

Even though crystallization is ubiquitous and has a potential field of applications, its fundamental mechanisms remain concealed. Then, a superior understanding is needed for satisfying potential applications in material science, biomedical, geology, and electronics [1, 2].

Although it is true that crystallization becomes challenging to simulate using Molecular Dynamics (MD) from liquids. Previous work as [3] has reported good results using crystal seeds. That is why we proposed to perform MD simulations around an artificial crystal seed, which would be complemented by experiments constructing seed structures of micrometric colloidal particles using optical tweezers.

To achieve this goal, we have used the hard-sphere model, i.e., we only consider the repulsive part of the potential; in this case, the Lennard-Jones potential. It is well-known that hard spheres result are a good approximation for colloidal particles. With the simulation, we will be able to identify the effects of crystal lattice spacing, crystal size, and density on the crystallization process in colloids.

2 Methods

Essentially, we have used two methods: *Radial distribution function* (RDF) and *bond-orientational order parameters* to recognize whether crystallization is occurring in our systems.

2.1 The Radial Distribution Function

Radial distribution function (RDF), usually denoted by $g(r)$, represents the probability to find an atom at the distance r of another atom chosen as a reference point [4].

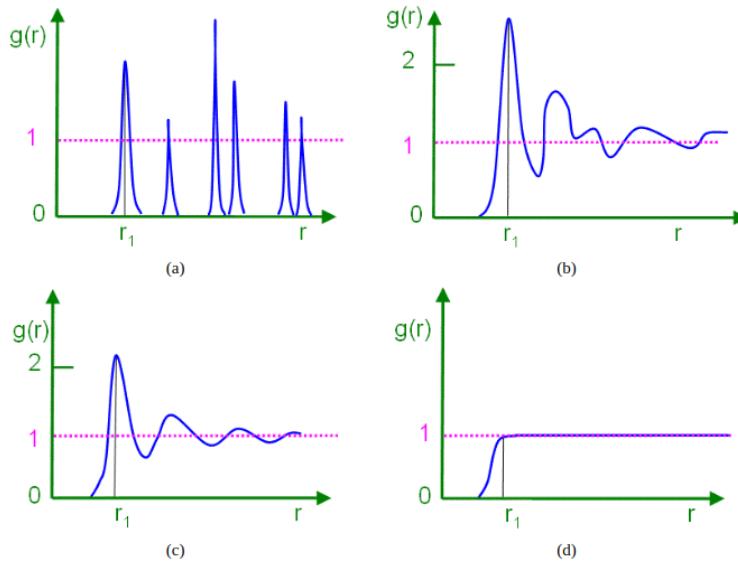


Figure 1: Illustration of RDF for (a) solid, (b) amorphous, (c) liquid, and (d) gas states. *Image taken from [4].*

2.2 Bond-orientational order parameters

Bond-orientational order can be used to identify hexagonal lattice in two-dimensional systems [5]. In this work, we have used the local order parameters proposed by Nelson and Halperin [6, 7] defined as:

$$q_n = \frac{1}{nnn} \sum_{j=1}^{nnn} e^{ni\theta(\mathbf{r}_{ij})} \quad (1)$$

where nnn is the number of the nearest neighbors of the selected atom, n is the degree of the order parameter, and $\theta(r_{ij})$ is the angle formed by the bond vector \mathbf{r}_{ij} and the x-axis.

For a perfect hexagonal lattice with $nnn = n = 6$ with an angle multiple of 60 degrees, getting:

$$q_6 = \frac{1}{6} \sum_{j=1}^6 e^{6i\frac{j\pi}{3}} = 1 \quad (2)$$

Is important, to mention that $q_6 = -1$ also represents a hexagonal lattice but with a different inclination. Then, if q_6 is close to zero means that the system has no hexagonal lattice, being likely a gas or liquid system. On the other hand, if q_6 is close to 1 (or -1), then the system is close to have a hexagonal lattice structure.

3 Simulation Details

For the Molecular Dynamics (MD) simulations, we have used the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) code [8]. For reading the output dump files, OVITO [9] was used as a viewer tool to do the respective analysis.

The main parameters used for MD simulations are:

- 2D hard-sphere model: Particles with a Lennard-Jones (LJ) repulsive potential.
- Lennard-Jones units [10]: All quantities are unitless, LAMMPS sets the fundamental quantities mass, σ, ϵ , and the Boltzmann constant $k_B = 1$.
- Canonical ensemble [11, 12]: This ensemble is highly useful for treating an actual experimental system that generally has a fixed V, N, and T.
- Small systems of about 1100 particles, and large systems of 10000 particles approximately.
- Time of 10^7 .
- Temperature of 0.025.
- LJ cutoff $= 2^{1/6}\sigma = 1.122$, having only the LJ repulsive potential [13].
- Different densities of colloidal from 0.5 to 0.8.
- Crystal seeds with 37, 55, 109, and 163 atoms.
- Crystals seeds with different lattice spacings from 1.1 to 1.9.

Before and after MD simulation

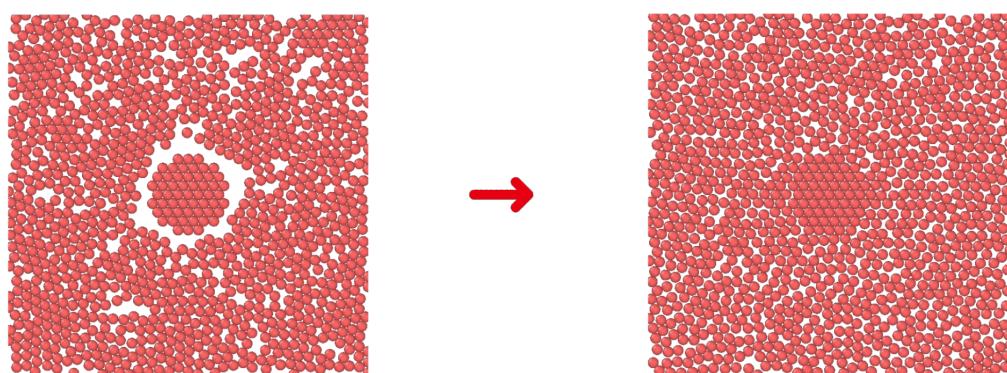


Figure 2: Small 2D system with a crystal seed made of 55 particles (a) before and (b) after the MD simulation.
Image viewed with OVITO [9].

4 Challenges

During this project some drawbacks appear, the most important ones were:

- RDF became a useful tool to prove and corroborate the LJ cutoff, and the general behavior of the systems, but not really useful to detect the hexagonal lattice of the systems.
- As a way to solve the previous difficulty, bond order parameters were used. The drawback presented was in the particles placed at the borders of the square box, and at the borders of the crystal seed. This happened because, as you may notice in eq. (1), as less than 6 neighbor particles around, the values will be close to zero. As you can see in Fig. 3, red color particles are values with q_6 values close to 1, whereas orange, yellow, and green are particles with q_6 values closer to zero respectively.
- The idea for solving these border effects was to increase the box size but maintain the same densities of the computed small boxes at that point. With larger systems, the statistics will correct this problem, giving as more accurate results. The crystallization in large boxes is more difficult to achieve but is a better approximation to real systems.
- Another problem was related to the hex/order command [7]. when, we tryed to get the q_6 values, we have chosen a radius = 2, but since we defined a LJ cutoff equal to $2^{1/6} = 1.12$ the code did not work. The solution was first running the MD simulation, and after that calculating the q_6 parameters just on a preferred time frame, in our case the last one.
- Finally, in larger systems, as I mentioned, crystallization was difficult to achieve and then many different variables were tested to improve this. For instance, we have increased time, densities, and lattice spacing in the crystal seed expecting an improvement, but as I will describe in the results section, this is only partially true.

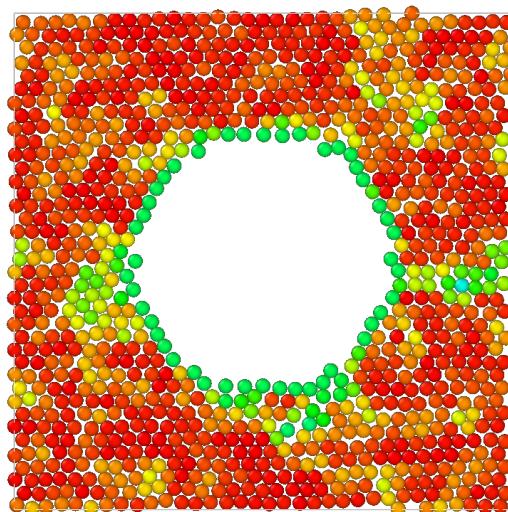


Figure 3: Problem with the bond order parameters at the edges. *Image viewed with OVITO [9].*

5 Small systems results

For the “small” systems, we have tested different densities of particles by varying the total number of particles (1175, 1100, 1025, and 875), and fixing a square box size of 40×40 .

Additionally, we have assessed three different sizes on the crystal seed with 55, 109, and 163 particles; and, for each crystal size, six variations of crystal seed lattice spacing were evaluated: 1.19, 1.30, 1.29, 1.38, 1.52, and 1.70. Pure liquid systems were also calculated using the corresponding densities, MD parameters, and the same methods.

5.1 Density = $1175/40 \times 40 = 0.734$

5.1.1 Crystal seed of 55 atoms

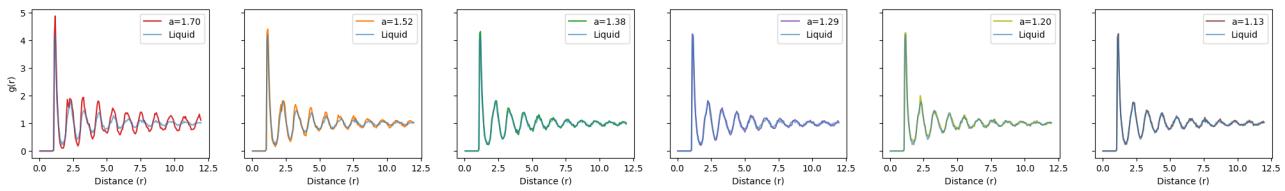


Figure 4: RDF of a system with a density of 0.734 using different lattice spacing for the crystal seed of 55 atoms.

According to the RDF plots, the first peak is $r = 1.12$ approximately, which is in agreement with the LJ cutoff we have defined. However, higher peak values than the liquid are only notable for 1.70 and 1.52. In the case of the other lattice spacings, RDFs are very similar to the pure liquid system.

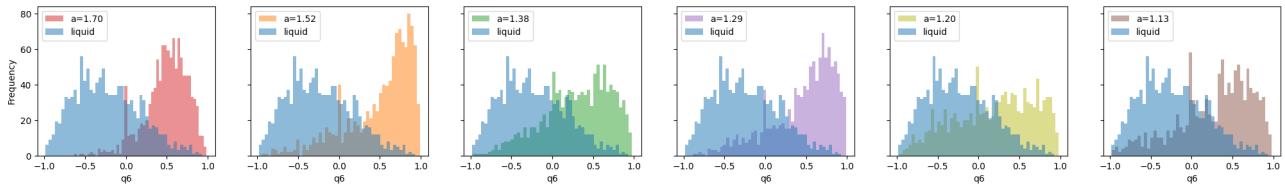


Figure 5: Hexatic bond order parameters of a system with a density of 0.734 using different lattice spacing for the crystal seed of 55 atoms.

Similarly, in the case of the hexatic order parameters, represented as histograms (Fig. 5) and colors (Fig. 6) show a notable improvement in crystallization for the systems with crystal seed lattice spacing of 1.70 and 1.52, but the other also show a better tendency to crystallization if it is compared with the liquid.

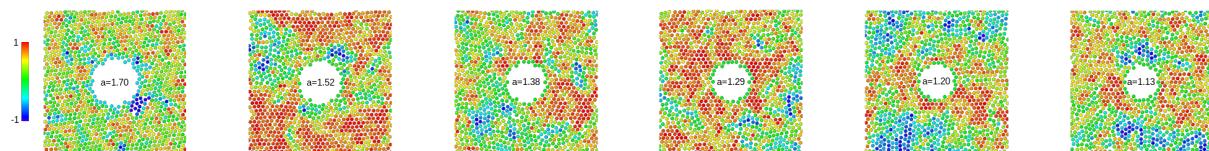


Figure 6: Small system with a density of 0.734 using different lattice spacing for the crystal seed of 55 atoms, where the colors represent the q_6 order parameters.

5.1.2 Crystal seed of 109 atoms

As depicted in Fig. 7, notable higher peak values for 1.70 and 1.52 as well as its whole behavior (not converging to one), gives us the information that these systems are highly crystallized.

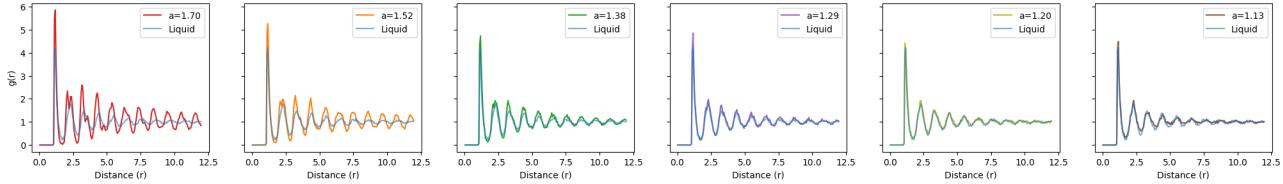


Figure 7: RDF of a system with a density of 0.734 using different lattice spacing for the crystal seed of 109 atoms.

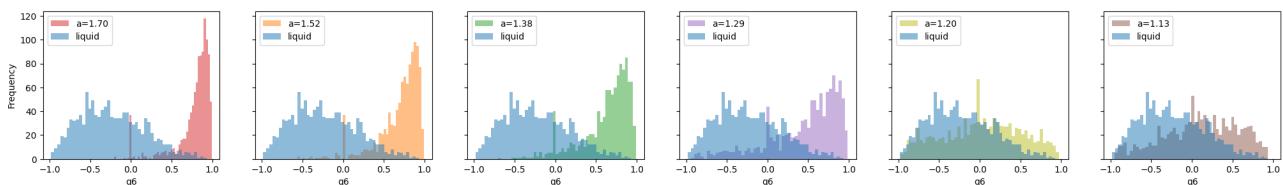


Figure 8: Hexatic bond order parameters of a system with a density of 0.734 using different lattice spacing for the crystal seed of 109 atoms.

In this same way, the hexatic order parameters showed a very high peak near 1 (Fig. 8), confirming the high crystallization that occurred in these systems, especially for 1.70 and 1.52 lattice spacings.

5.1.3 Crystal seed of 163 atoms

Increasing the crystal seed has shown to be an effective way to improve crystallization. That is the reason why we have calculated this case.

Fig. 9 shows a huge enhancement of crystallization compared with the previous crystal sizes. A curious effect happened for the systems with a lattice spacing of 1.70, which preferred to crystallize with a different inclination, going the q_6 to -1 as you can see in Fig. 10. We inferred this could be due to an excessive density.

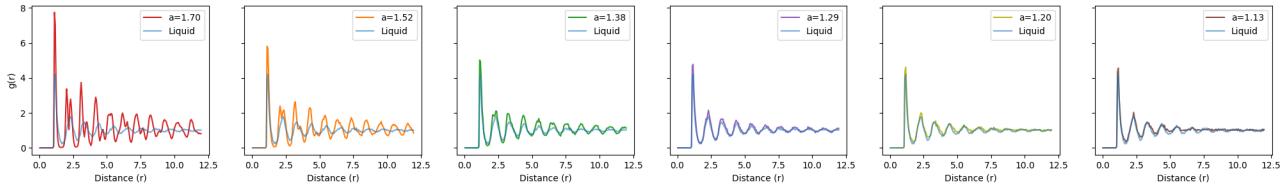


Figure 9: RDF of a system with a density of 0.734 using different lattice spacing for the crystal seed of 163 atoms.

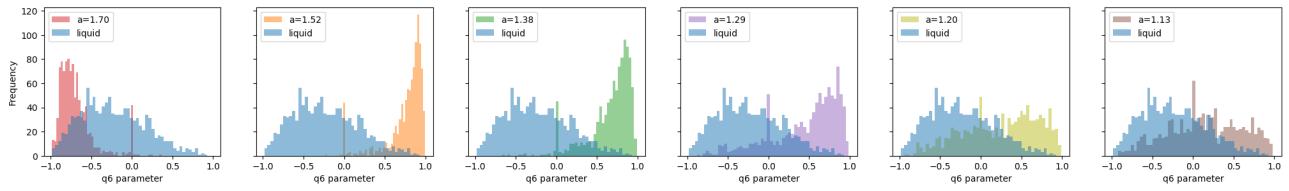


Figure 10: Hexatic bond order parameters of a system with a density of 0.734 using different lattice spacing for the crystal seed of 109 atoms.

5.2 Density = $1100/40 \times 40 = 0.687$

5.2.1 Crystal seed of 55 atoms

Figure 39 shows no significant changes in the systems with the crystal seed in comparison with the pure liquid, giving us an idea that systems did not achieve any crystallization.

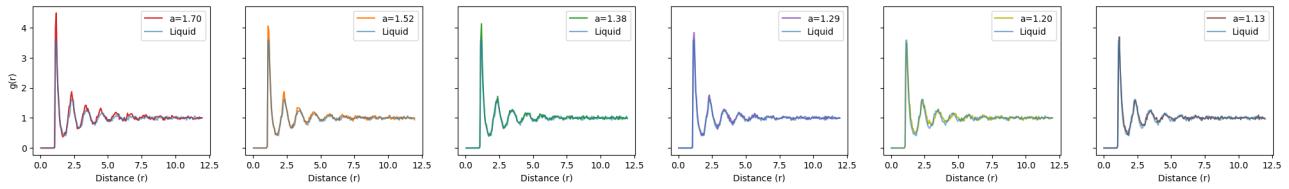


Figure 11: RDF of a system with a density of 0.687 using different lattice spacing for the crystal seed of 55 atoms.

In the same manner, the q_6 parameters shown in Fig. 40 just confirm there is not enough crystallization in the proposed systems.

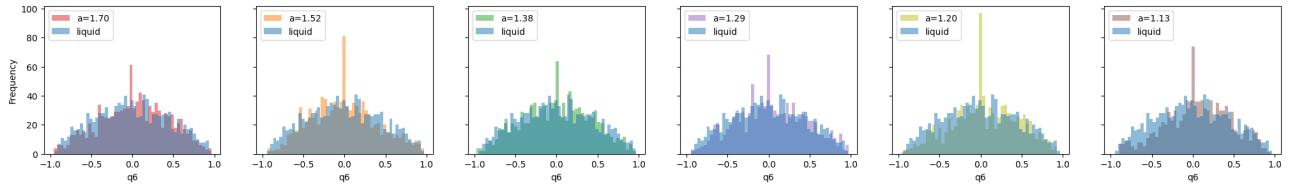


Figure 12: Hexatic bond order parameters of a system with a density of 0.687 using different lattice spacing for the crystal seed of 55 atoms.

5.2.2 Crystal seed of 109 atoms

Increasing the crystal seed to 109 as you can notice in Figure 41, there are some peaks for the higher lattice spacings, which means there could be some crystallization there.

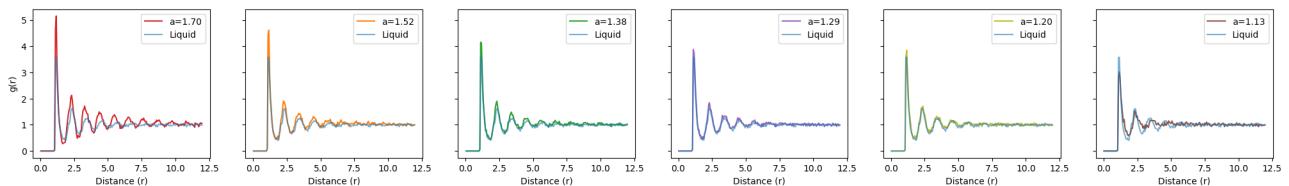


Figure 13: RDF of a system with a density of 0.687 using different lattice spacing for the crystal seed of 109 atoms.

However, the q_6 parameters are clear, showing in my opinion, there is not enough crystallization again.

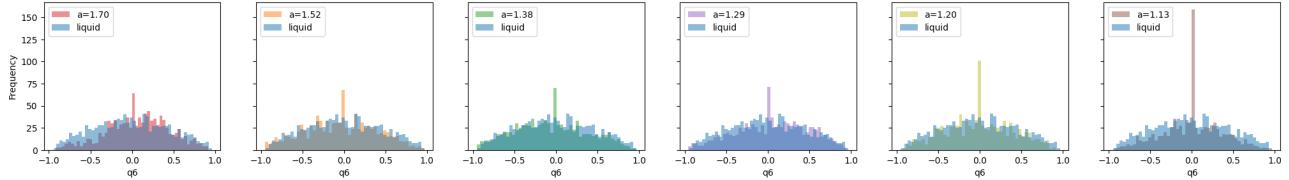


Figure 14: Hexatic bond order parameters of a system with a density of 0.687 using different lattice spacing for the crystal seed of 109 atoms.

5.2.3 Crystal seed of 163 atoms

Figure 15 shows a significant improvement in the crystallization, at least for the lattice spacings 1.70 and 1.50.

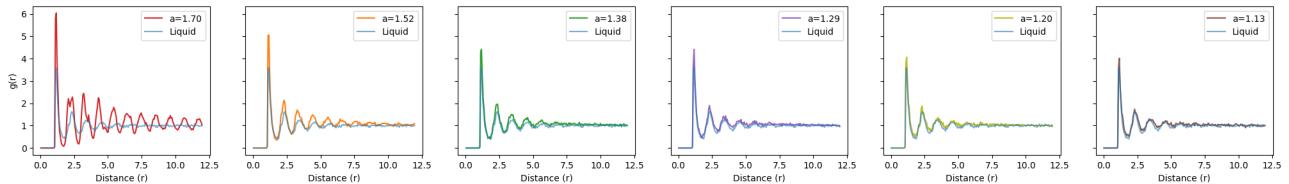


Figure 15: RDF of a system with a density of 0.687 using different lattice spacing for the crystal seed of 163 atoms.

Even though the q_6 parameters (Fig. 16) show a slight boost in crystallization, there is not enough to state these systems are good candidates for our goals.

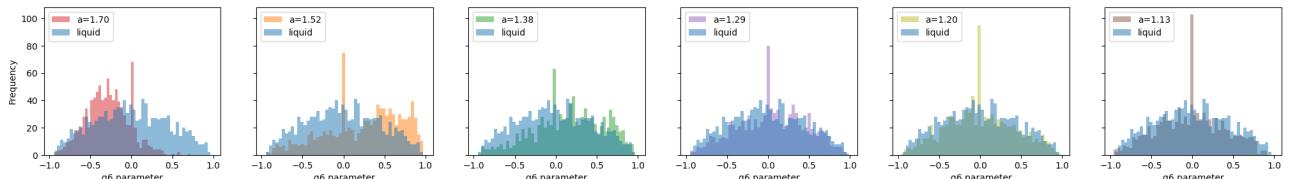


Figure 16: Hexatic bond order parameters of a system with a density of 0.687 using different lattice spacing for the crystal seed of 163 atoms.

5.3 Density = 1025/40×40 = 0.640

5.3.1 Crystal seed of 55 atoms

As we expected, Fig. 17 shows no significant changes in the systems with the crystal seed in comparison with the pure liquid.

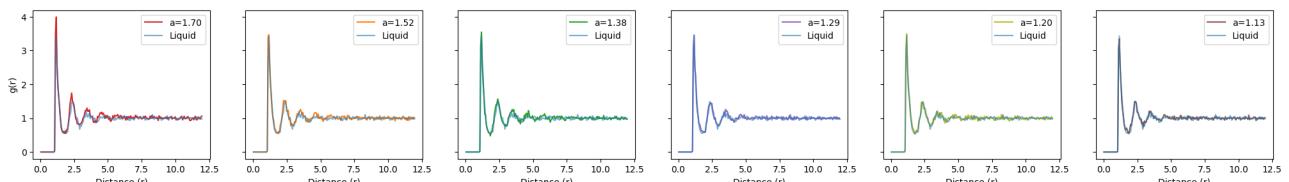


Figure 17: RDF of a system with a density of 0.640 using different lattice spacing for the crystal seed of 55 atoms.

In the same manner, the q_6 parameters shown in Fig. 18 the lack of crystallization in the proposed systems.

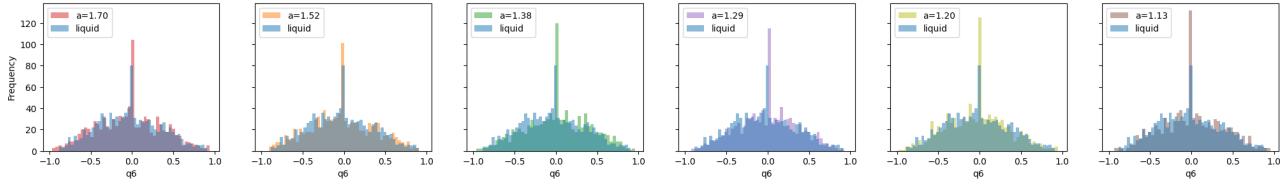


Figure 18: Hexatic bond order parameters of a system with a density of 0.640 using different lattice spacing for the crystal seed of 55 atoms.

5.3.2 Crystal seed of 109 atoms

Increasing the crystal seed to 109 has slightly increased some peaks (Fig. 19) for the higher lattice spacings.

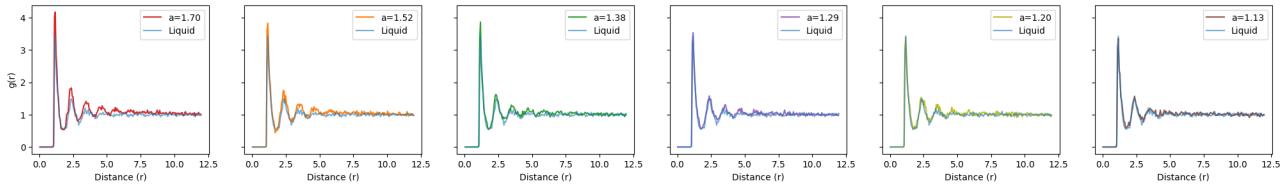


Figure 19: RDF of a system with a density of 0.640 using different lattice spacing for the crystal seed of 109 atoms.

However, q_6 parameters show clearly that there is not enough crystallization again.

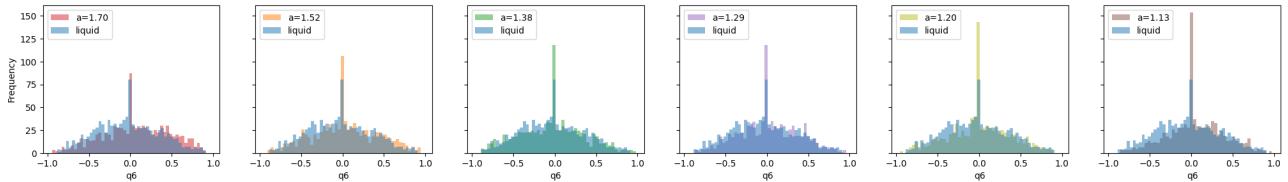


Figure 20: Hexatic bond order parameters of a system with a density of 0.640 using different lattice spacing for the crystal seed of 109 atoms.

5.3.3 Crystal seed of 163 atoms

Figure 21 shows a significant improvement in the crystallization, at least for the lattice spacings 1.70 and 1.50. But is not enough as showed in Fig. 22.

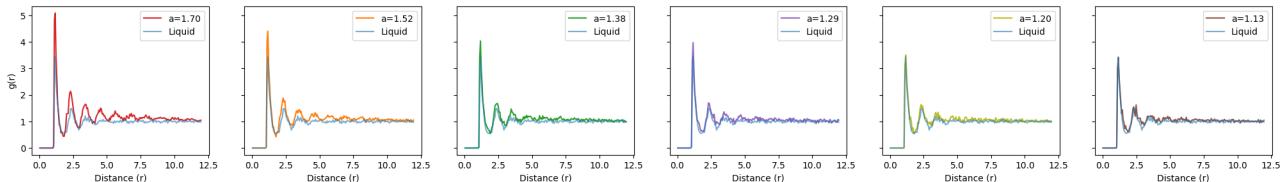


Figure 21: RDF of a system with a density of 0.640 using different lattice spacing for the crystal seed of 163 atoms.

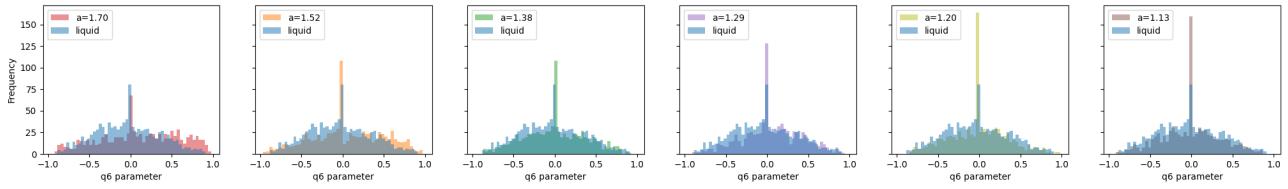


Figure 22: Hexatic bond order parameters of a system with a density of 0.640 using different lattice spacing for the crystal seed of 163 atoms.

5.4 Densities lower than 0.640

We have carried MD simulations out of systems with lower densities than 0.640 such as 0.546, but there did not show crystallization. Then, for future studies, we suggest taking into account that lower densities are not appropriate.

5.5 Final Analysis: RDF vs Seed Size

Our coordination analysis calculations go from $r = 0$ to $r = 12$. Then, for this analysis, a small range in the x-axis (from 7.23 to 8.43) was selected in order to get the maximum peak of $g(r)$. If the value is close to one, it means it is closer to being a liquid. On the other hand, if the value is bigger than 1, it could be proof of crystallization. However, as we showed previous results, a bond order analysis is needed to affirm this.

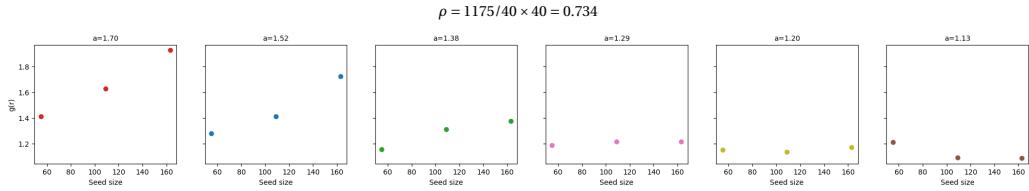


Figure 23: Seed size vs $g(r)$ for small systems with a density of 0.734. Note that for the biggest lattice spacings, 1.70 and 1.52, there is a clear linear tendency; in other words, the crystallization improves linearly as we increase the crystal seed size.

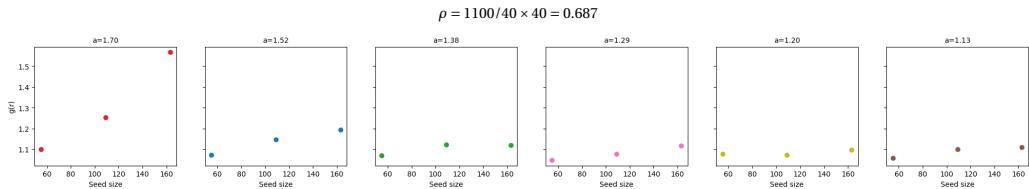


Figure 24: Seed size vs $g(r)$ for small systems with a density of 0.687. Note that, in this case, only for the biggest lattice spacing, 1.70, there is a linear increment of the RDF; in other words, the crystallization improves linearly as we increase the crystal seed size.

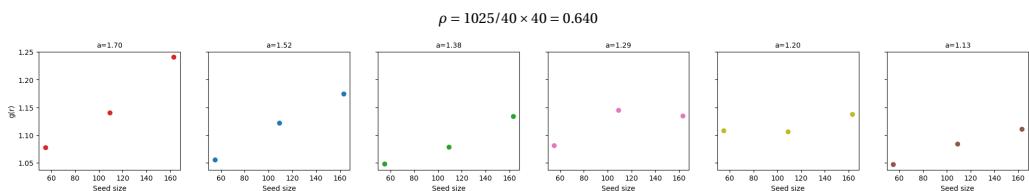


Figure 25: Seed size vs $g(r)$ for small systems with a density of 0.640. In this case, the lattice spacing 1.70 should be analyzed in detail, we cannot ensure a good linear trend because the increment in $g(r)$ is perhaps not enough.

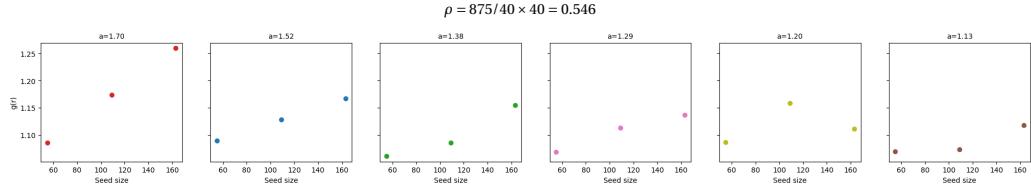


Figure 26: Seed size vs $g(r)$ for small systems with a density of 0.640. In this case, we cannot ensure a good linear trend because the increment in $g(r)$ is perhaps not enough.

5.6 Final Analysis: RDF vs Lattice Spacing

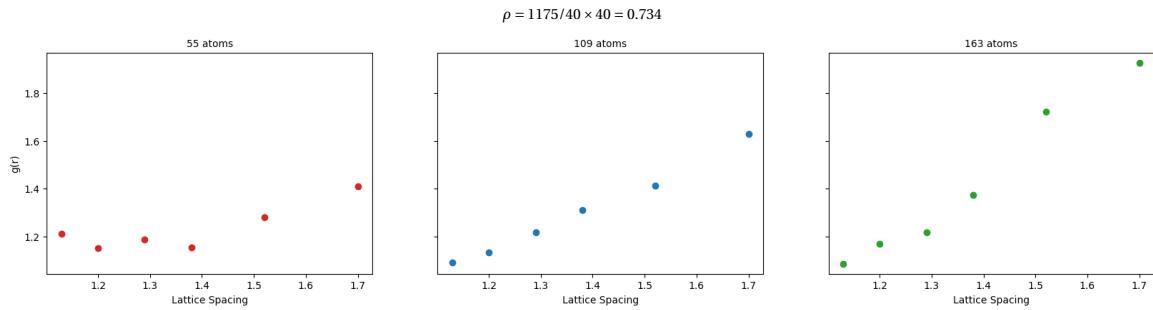


Figure 27: Lattice spacing vs $g(r)$ for small systems with a density of 0.734. In this case, a crystal seed of 163 and 190 atoms are the best options for improving crystallization; showing a high linear increment as the lattice spacing increases. A crystal seed made of 55 atoms is not good enough.

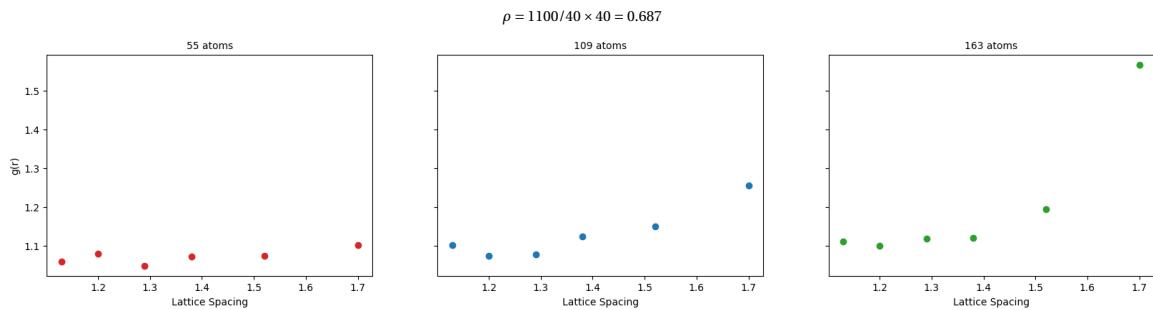


Figure 28: Lattice spacing vs $g(r)$ for small systems with a density of 0.687. In this case, a crystal seed of 163 is still a good candidate for improving crystallization; showing a high linear increment as the lattice spacing increases. The other two crystal seed made of 55 and 109 atoms are not good enough.

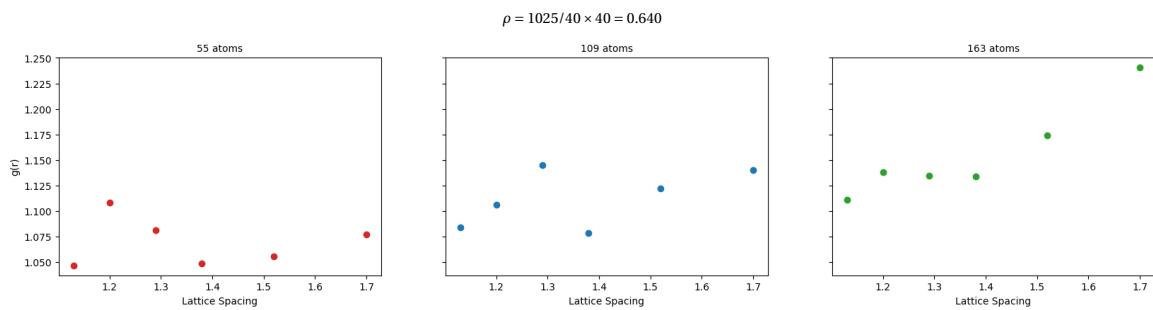


Figure 29: Lattice spacing vs $g(r)$ for small systems with a density of 0.640. In this case, a crystal seed of 163 is not too practical to produce crystallization. Lower crystal seed sizes are not appropriate.

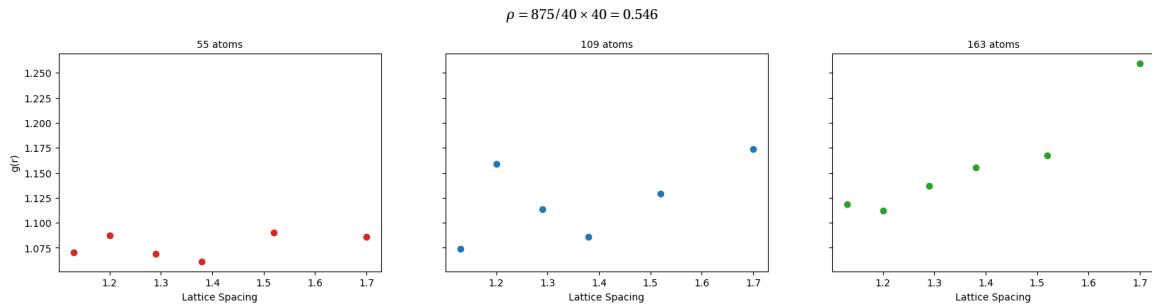


Figure 30: Lattice spacing vs $g(r)$ for small systems with a density of 0.546. Any of the three crystal seeds are a good choice to produce crystallization.

6 Large Systems Results

For the “large” systems, we have repeated the two higher densities of the calculated “small” systems which showed to have a potential enhancement in crystallization. That is to say, we have calculated two systems with 10000 and 9359 number of particle, and with a fixed squared box size of 116.72×116.72 .

Additionally, we have received a recommendation of avoiding calculated systems with high crystal size because, in a real experiment, this will be very tough to achieve. Then, we have not used the 163 atoms crystal seed anymore, instead, we created a crystal seed of 37 atoms.

In the same manner, we did not repeat the small lattice spacings, 1.13 nor 1.20 but we add a new higher lattice spacing equal to 1.96.

6.1 Density = $10000/116.72 \times 116.72 = 0.734$

6.1.1 Crystal seed of 37 atoms

Figure 31 shows the very similar behavior of the RDF between the pure liquid system and one with a crystal seed of 37 atoms, i.e. the crystal seed seems not to have a good effect in the crystallization.

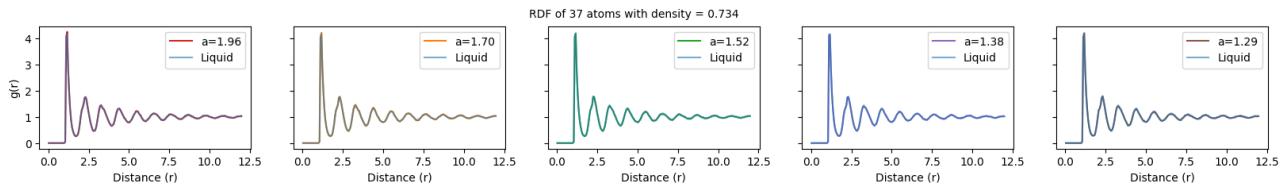


Figure 31: RDF of a system with a density of 0.734 using different lattice spacing for the crystal seed of 37 atoms.

The hexatic bond parameters confirm the behavior of the crystal seed systems that we suspect analyzing the RDF, there is no significant crystallization as you can see in Fig. 32

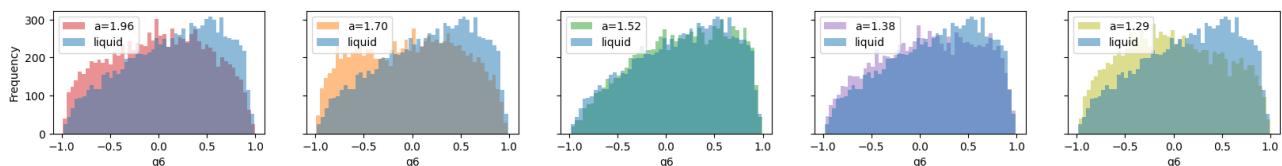


Figure 32: Hexatic bond order parameters of a system with a density of 0.734 using different lattice spacing for the crystal seed of 37 atoms.

6.1.2 Crystal seed of 55 atoms

Figure 33 also shows a similar behavior of the RDF between the pure liquid system and one with a crystal seed of 55 atoms.

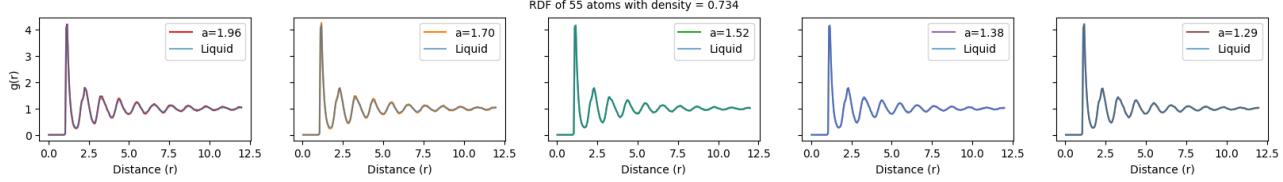


Figure 33: RDF of a system with a density of 0.734 using different lattice spacing for the crystal seed of 55 atoms.

Even though Fig. 34, the hexatic bond parameters, show that systems with a crystal seed with lattice spacings of 1.96 and 1.70 have crystallization there is no immense difference with the pure liquid as the difference we saw in the small systems. Taking into account, that in the small systems, the good choices with this density and crystal seed were 1.70 and 1.52. This time 1.52 is not a good choice anymore.

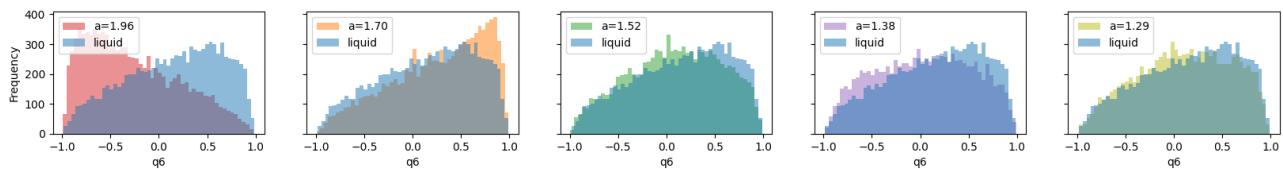


Figure 34: Hexatic bond order parameters of a system with a density of 0.734 using different lattice spacing for the crystal seed of 55 atoms.

6.1.3 Crystal seed of 109 atoms

The RDF figures still show a strong similitude between the pure liquid and the one with the crystal seed (Fig. 35). However, Fig. 36, shows that system with a crystal seed with a lattice spacing of 1.96 is a potential candidate to improve crystallization.

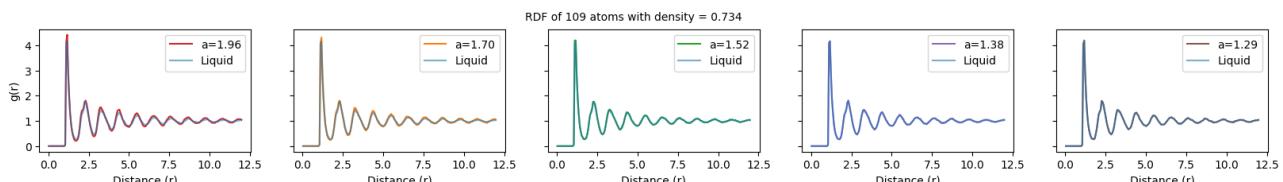


Figure 35: RDF of a system with a density of 0.734 using different lattice spacing for the crystal seed of 109 atoms.

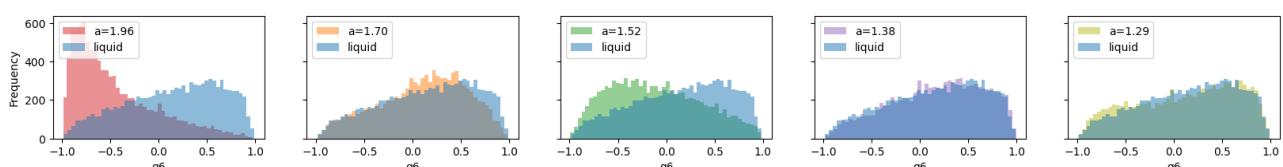


Figure 36: Hexatic bond order parameters of a system with a density of 0.734 using different lattice spacing for the crystal seed of 109 atoms.

6.2 Density = 9359/116.72×116.72 = 0.687

Unfortunately, all the systems with this density did not show enough crystallization.

6.2.1 Crystal seed of 37 atoms

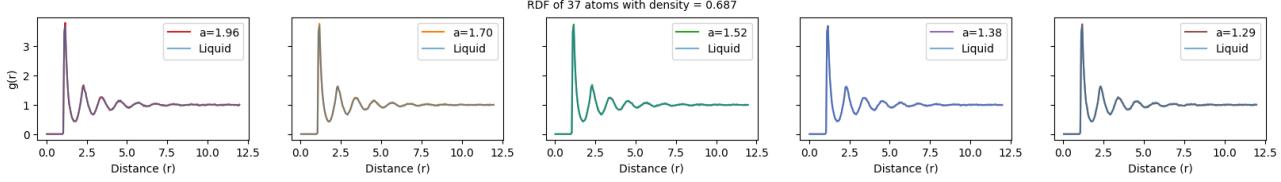


Figure 37: RDF of a system with a density of 0.687 using different lattice spacing for the crystal seed of 37 atoms.

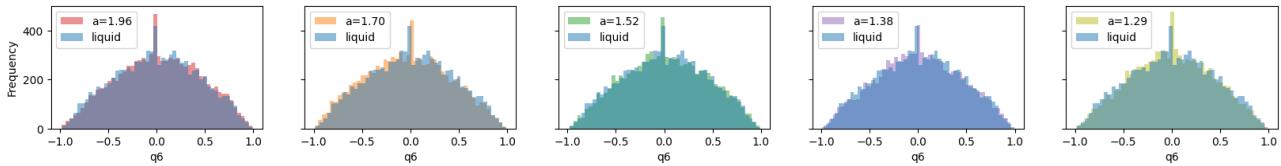


Figure 38: Hexatic bond order parameters of a system with a density of 0.687 using different lattice spacing for the crystal seed of 37 atoms.

6.2.2 Crystal seed of 55 atoms

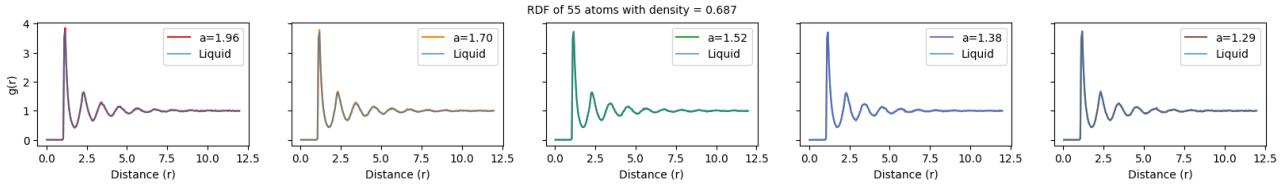


Figure 39: RDF of a system with a density of 0.687 using different lattice spacing for the crystal seed of 55 atoms.

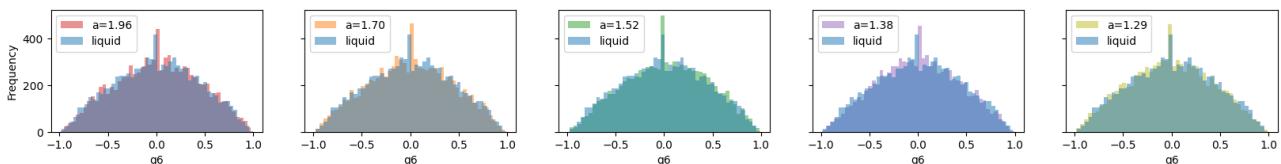


Figure 40: Hexatic bond order parameters of a system with a density of 0.687 using different lattice spacing for the crystal seed of 55 atoms.

6.2.3 Crystal seed of 109 atoms

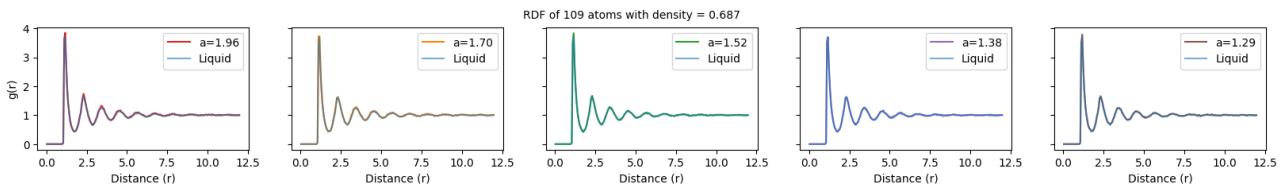


Figure 41: RDF of a system with a density of 0.687 using different lattice spacing for the crystal seed of 109 atoms.

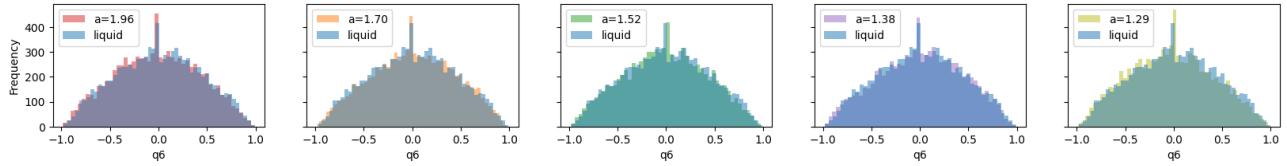


Figure 42: Hexatic bond order parameters of a system with a density of 0.687 using different lattice spacing for the crystal seed of 109 atoms.

6.3 Looking for crystallization in large systems with a crystal seed of 37 atoms

We did not encounter an enhancement of crystallization using a crystal seed of 37 atoms. That is the reason why we focus on finding the critical density at which the crystallization may occur in these systems.

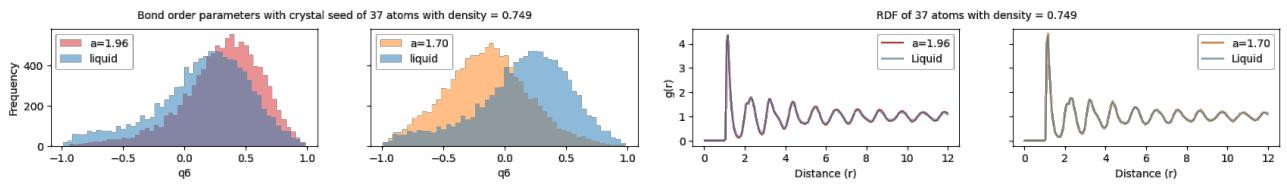


Figure 43: The first trial of getting crystallization, was to increase the density to 0.749 with the two highest lattice spacing of the crystal seed of 37 atoms.

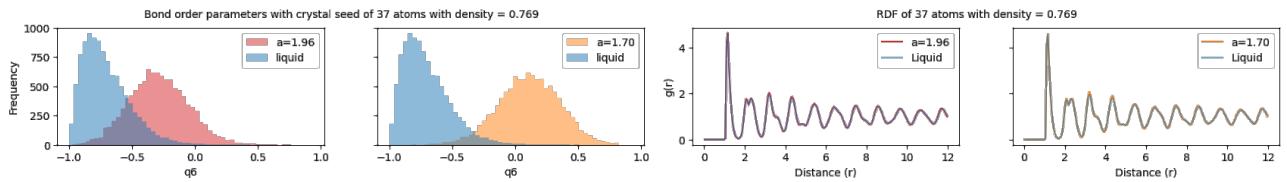


Figure 44: The second trial of getting crystallization, was to increase the density to 0.769 with the two highest lattice spacing of the crystal seed of 37 atoms.

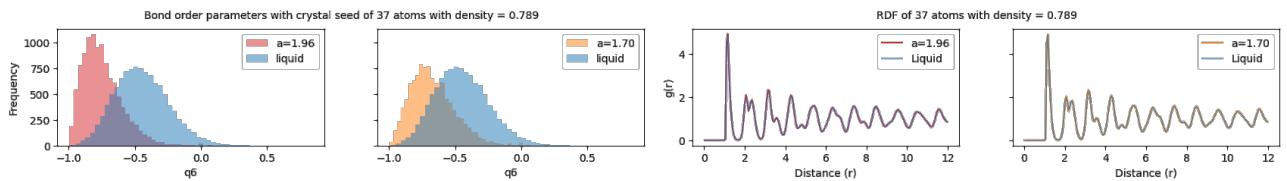


Figure 45: The final trial of getting crystallization, was to increase the density to 0.789 with the two highest lattice spacing of the crystal seed of 37 atoms.

A strange behavior we encounter was the system with a density of 0.769, where the pure liquid system showed more crystallization than the one with the crystal seed made of 37 atoms.

According to the results, a crystal seed of 37 does not have a consequential effect on crystallization.

6.4 Final Analysis: RDF vs Seed Size

The same analysis made for the small systems was made here. Since coordination analysis calculations go from $r = 0$ to $r = 12$; then, for this analysis, a small range in the x-axis (from 7.23 to 8.43) was selected in order

to get the maximum peak of $g(r)$. If the value is close to one, it means it is closer to being a liquid. On the other hand, if the value is bigger than 1, it could be proof of crystallization. However, as we showed previous results, a bond order analysis is needed to affirm this.

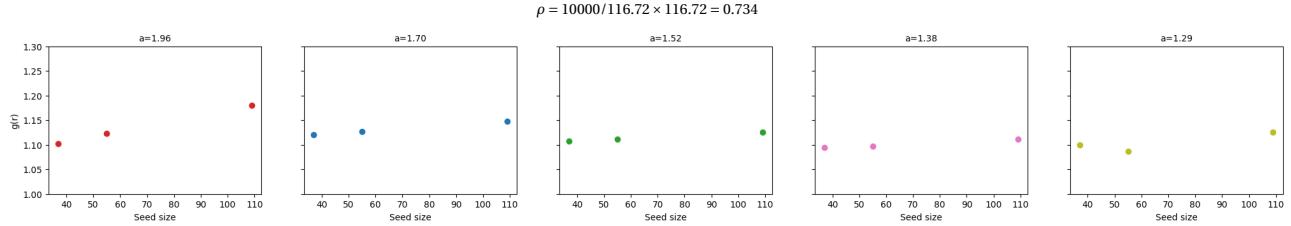


Figure 46: Seed size vs $g(r)$ for large systems with a density of 0.734. Note that there is a linear increasing trend for the systems, but only the biggest crystal seed lattice spacing shows an appreciable increment in the $g(r)$ as we increase the crystal size.

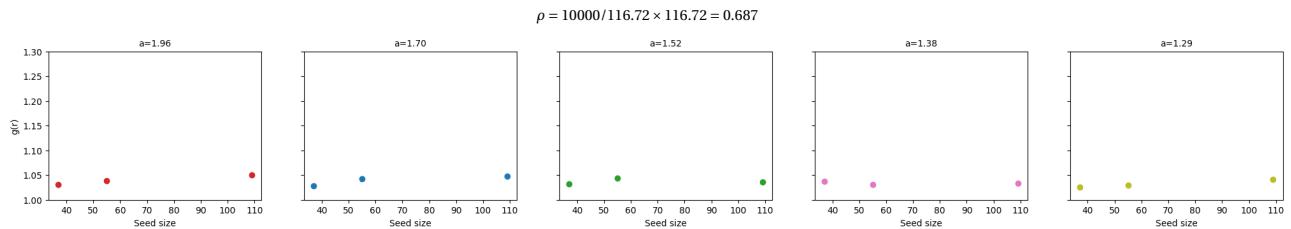


Figure 47: Seed size vs $g(r)$ for large systems with a density of 0.687. Note that there is no good enough increment as we increase the lattice spacing of the crystal size.

6.5 Final Analysis: RDF vs Lattice spacing

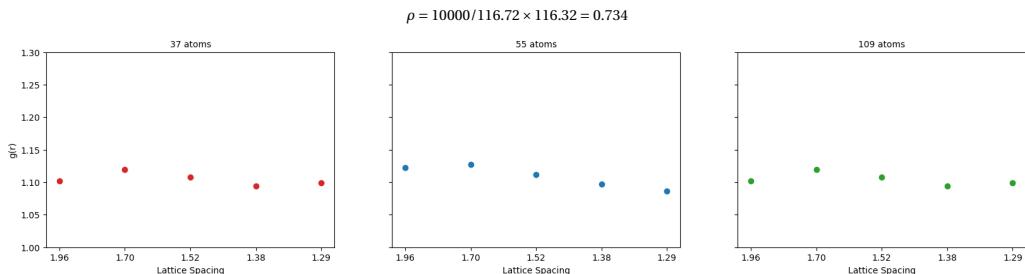


Figure 48: Lattice spacing vs $g(r)$ for large systems with a density of 0.734. Any case shows a good tendency as we increase the lattice spacing in the crystal seed.

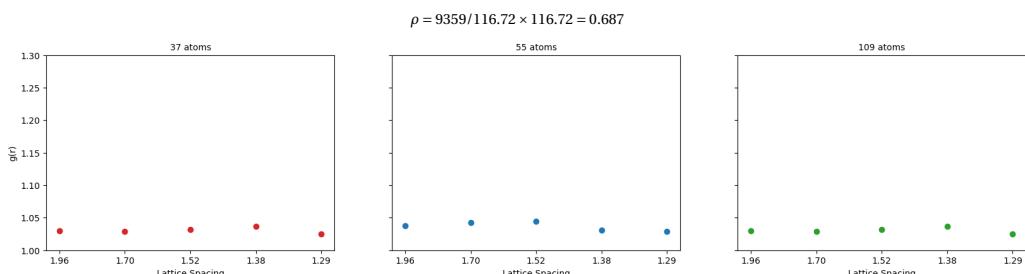


Figure 49: Lattice spacing vs $g(r)$ for large systems with a density of 0.687. Any case shows a good tendency as we increase the lattice spacing in the crystal seed.

7 Conclusions

- Small systems tend to overestimate crystallization because of confined effects.
- Large systems gave us more realistic results; realizing that crystallization is difficult to achieve with the proposed parameters.
- A crystal seed of 37 atoms is not large enough to enhance crystallization in large systems, for example, 10000 particles.
- Densities larger than 0.8 were inappropriate since outside particles got stuck with to without a crystal seed.
- In the same way, larger lattice distances than 1.96 were proved, but there were no good choices because particles of the liquid started to come through the seed.
- Increasing time to 10^9 did not show an improvement in crystallization.
- The most promising system configuration we find is a density of 0.734, using a crystal seed with a lattice spacing of 1.96. We are sure it will improve by increasing the crystal seed size, but this could be hard to achieve experimentally.

Acknowledgements

I would like to thank Prof. Julien Lam for allowing me to join this interesting project. Also, I would like to thank Akshay Ammothum, Ph.D. for the fruitful discussions and for his patient during the project.

References

- [1] K. An and T. Hyeon, "Synthesis and biomedical applications of hollow nanostructures," *Nano Today*, vol. 4, no. 4, pp. 359–373, 2009.
- [2] N. Gaponik, S. G. Hickey, D. Dorfs, A. L. Rogach, and A. Eychmüller, "Progress in the light emission of colloidal semiconductor nanocrystals," *small*, vol. 6, no. 13, pp. 1364–1378, 2010.
- [3] M. Hermes, E. Vermolen, M. Leunissen, D. Vossen, P. Van Oostrum, M. Dijkstra, and A. Van Blaaderen, "Nucleation of colloidal crystals on configurable seed structures," *Soft Matter*, vol. 7, no. 10, pp. 4623–4628, 2011.
- [4] J. Lu and J. A. Szpunar, "Applications of the embedded-atom method to glass formation and crystallization of liquid and glass transition-metal nickel," *Philosophical Magazine A*, vol. 75, no. 4, pp. 1057–1066, 1997.
- [5] P. J. Steinhardt, D. R. Nelson, and M. Ronchetti, "Bond-orientational order in liquids and glasses," *Physical Review B*, vol. 28, no. 2, p. 784–805, 1983.
- [6] D. R. Nelson and B. I. Halperin, "Dislocation-mediated melting in two dimensions," *Physical Review B*, vol. 19, no. 5, p. 2457, 1979.
- [7] "Compute hexorder/atom command." https://docs.lammps.org/compute_hexorder_atom.html.
- [8] A. P. Thompson, H. M. Aktulga, R. Berger, D. S. Bolintineanu, W. M. Brown, P. S. Crozier, P. J. in 't Veld, A. Kohlmeyer, S. G. Moore, T. D. Nguyen, R. Shan, M. J. Stevens, J. Tranchida, C. Trott, and S. J. Plimpton, "LAMMPS - a flexible simulation tool for particle-based materials modeling at the atomic, meso, and continuum scales," *Comp. Phys. Comm.*, vol. 271, p. 108171, 2022.
- [9] A. Stukowski, "Visualization and analysis of atomistic simulation data with ovito—the open visualization tool," *Modelling and Simulation in Materials Science and Engineering*, vol. 18, no. 1, p. 015012, 2009.
- [10] "Units command." <https://docs.lammps.org/units.html>.
- [11] A. Satoh, "Statistical ensembles," *Introduction to Molecular-Microsimulation of Colloidal Dispersions*, p. 7–18, 2003.
- [12] "Fix nvt command." https://docs.lammps.org/fix_nh.htm.
- [13] "Pair style lj/cut command." url=https://docs.lammps.org/pair_lj.html.