Phase Transition and Morphological Analysis of 2D-Colloidmonolayer

Quest project of Niels Schalenberg

Introduction

- Colloidal spheres serve as model systems in condensed matter for polymers, bacteria , fluid dynamics and many more
- 2D Layers enable direct visualization and particle tracking, making Monolayers ideal testing grounds for structural analyses
- Morphological analysis then reveals how molecular motion causes collective behaviour and structure forming
- Enables quantitative detection of particle distribution, ordering, lattice defects, lattice structures and phase transitions

Research Question

- **How can you measure order an a molecular level?**
- Consider a 2D layer of colloidal spherical particles
- Using Molecular Dynamic-simulations for the liquid-crystal transition by increasing the density of the layer

  Liquid = Disordered | Crystal lattice = Ordered
- Implement various functions to describe the local and system wide order after simulating

Result 1: Neighbour Defect Analysis

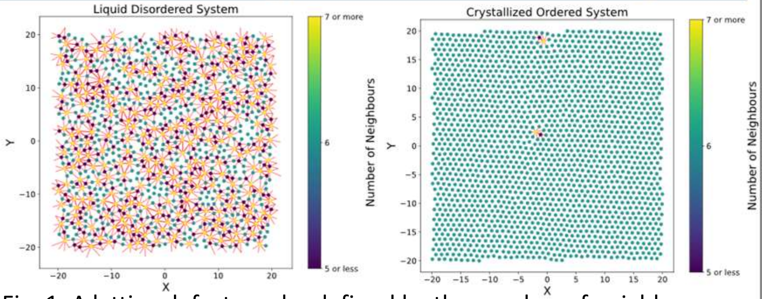

Fig. 1. A lattice defect can be defined by the number of neighbours surrounding a particle. Showing if particles are evenly distributed.

Neighbours calculated using Delauney Triangulation [2]

- Local order through absence of defects
- Displays particle position
- Line-defects for interfaces with subcrystals

Result 2: Order Parameter Ψ

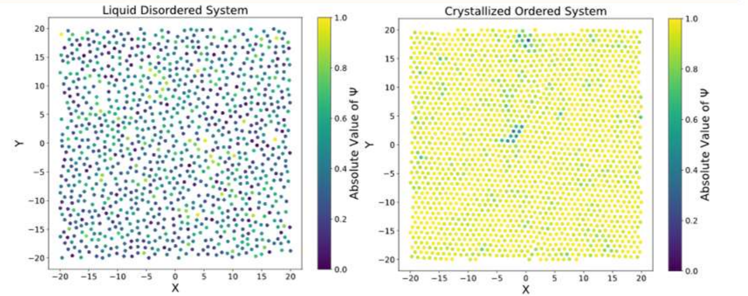

Fig. 2: The local orientational bond order parameter evaluates how well the neighbours are aligned, compared to the hexagonal shape.

$$\Psi_6 = \frac{1}{N}\sum_{j=1}^{N} e^{6i\theta_\mathrm{j}}$$

N = Number of Neighbours
θ = Neighbour orientation angle

- Local order through alignment $|\Psi|$
- Displays particle position
- Complex Angle of Ψ gives lattice orientation [1]

Result 3: Scattering Function and Circular Averaged Scattering Function

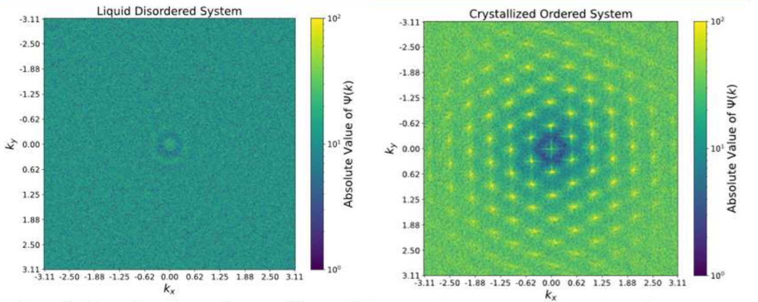

Fig. 3: Fourier transformation of the Order Parameter distribution..

$\Psi(\widetilde{\mathrm{k_x}, \mathrm{k_y}})$ = The Fourier Transformation of $\Psi(\mathrm{x}, \mathrm{y})$

- Global order by tendency to lattice formation
- Determines lattice type
- Indicates lattice orientation

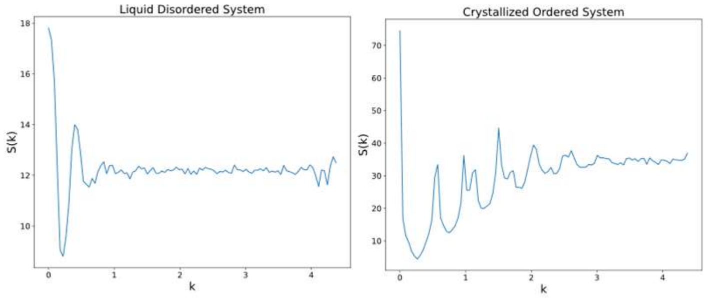

Fig. 4: Circular average of the Fourier Transformation above. Sharp peaks indicate periodic structure

$$\mathrm{S(k)} = \langle \Psi(\boldsymbol{k})\Psi(\boldsymbol{k})^* \rangle$$
$$\Psi(\mathbf{k}) = \Psi(\widetilde{\mathrm{k_x}, \mathrm{k_y}})$$ [1]

- Global order by definition of peaks
- Indicates how long ranged the local order is
- Determines lattice type by characteristic peaks

Result 4: Pair Distribution Function

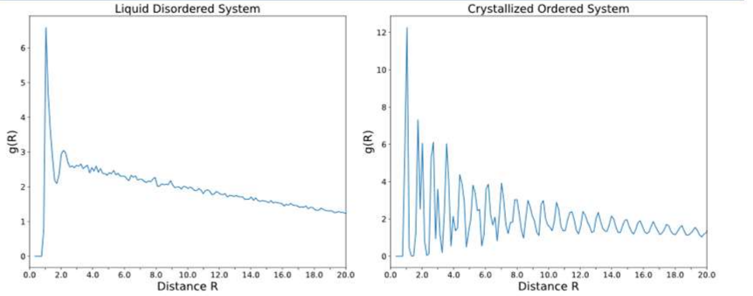

Fig. 5: Distribution of particle pairs with distance R to each other.

$$g(\mathrm{R}) = \frac{A_{Box}}{N(N-1)} \frac{\sum_{i=1}^{N}\sum_{j=i+1}^{N} \delta\{(\mathrm{R}-\epsilon) < r_{ij} < (\mathrm{R}+\epsilon)\}}{\pi\left((\mathrm{R}-\epsilon)^2 - (\mathrm{R}+\epsilon)^2\right)}$$

N = Number of particles
A = Area of simulation Box

- Global Order by definition of peaks [2]
- Indicates how long ranged local order is

Conclusion and Outlook

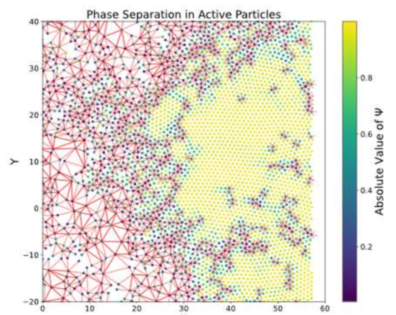

Fig. 6: Defects and order of a phase separation with driven particles.

- Local and global order establish for packing fractions above 0.75
- The collective results are able to describe occurring structure and order
- Quasi-long ranged hexatic phase for packing fractions between 0.75-0.8
- Able to show appearance of defects in otherwise ordered assemblies for active particles

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QUEST

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[1] Daniel A. Vega, Christopher K. Harrison, Dan E. Angelescu, Matthew L. Trawick, David A. Huse, Paul M. Chaikin, and Richard A. Register. **Ordering mechanisms in two-dimensional sphere-forming block copolymers**. Phys. Rev. E, 71:061803, Jun 2005.

[2] Valeria Lotito and Tomaso Zambelli. **Pattern detection in colloidal assembly: A mosaic of analysis techniques**. Advances in Colloid and Interface Science, 284:102252, 2020.