

TP Bubble Raft - *sur place*

Completing this TP should allow you to:

- Distinguish between different types of defects that can appear in two dimensions.
- Develop understanding of the nature of dislocations.
- Understand the motion of dislocations under an applied stress.

What is expected from you:

- To make a video that summarizes your observations of different lattice defects, including the response of the raft to the external stress.

The first theory that described the elastic fields of a material with *distortions* ("les distortions") was originally developed by Vito Volterra in his 1907 thesis [3]. In the years to follow one of the biggest challenges in materials science was to explain plasticity of materials from microscopic point of view. A simple back-of-the-envelope calculation of the **shear stress** at which neighboring planes of atoms of a perfect crystalline material **slip** over each other, would predict that metals have shear stresses of 3000 – 24000 MPa, where actual measurements would give a range of 0.5 – 10 MPa.

It was not until 1930s that an explanation was proposed. The term **dislocation**, meaning a **defect or irregularity on the atomic scale**, was first introduced by G. I. Taylor in 1934 [2], and in the same year E. Orowan, M. Polanyi and G. I. Taylor independently proposed that plastic deformation could be explained in terms of the theory of dislocations. It was proposed that dislocations move if the atoms from one of the surrounding planes break their bonds and reform them with the atoms at the terminating edge. And a half plane of atoms is moved in response to shear stress by breaking and reforming a line of bonds, one (or a few) at a time. The energy required to break a row of bonds is far less than that required to break all the bonds on an entire plane of atoms at once. This simple model suggested that that plasticity is possible at much lower stresses than in a perfect (defect-free) crystal. (Today we know that in many materials, particularly ductile materials, dislocations are the *carriers* of plastic deformation, and the energy required to move them is less than the energy required to fracture the material itself). The model also suggested an explanation of why materials work-harden, i.e., when a material has been plastically deformed, afterwards it requires greater stress to deform further.

It wasn't until 1947 that the existence of dislocations was experimentally verified. In their model system of mono-disperse air bubbles floating on a liquid surface, i.e., a **bubble raft** (see figure 1), W. L. Bragg and J. F. Nye demonstrated how defects, i.e., different imperfections of a lattice including the aforementioned dislocations, form, move and interact [1]. It took another ten years before electron microscopy techniques were advanced enough to show dislocations moving through a material.

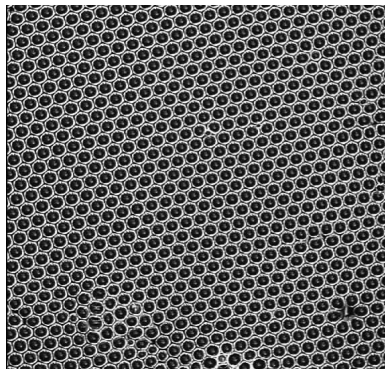


Figure 1: A top view of a bubble raft.

This TP

In this TP you will recreate the experiment of Bragg and Nye, i.e., you will create a bubble raft and use it to visualise how defects interact with each other, how they move and how they can be destroyed.

If the bubbles are small (1mm) and are mono-disperse, the raft is a very good two dimensional model of a crystal - the regular arrangement of the bubbles is an analogue to the structure of a close packed plane of atoms in e.g. aluminium. **The defects** in the arrangement of bubbles are closely analogous to such features in real crystalline materials. You will focus on *grain boundaries* (see figure 2), on *point defects* (see figure 3) and on *lattice dislocations* (see figures 3 and 4).

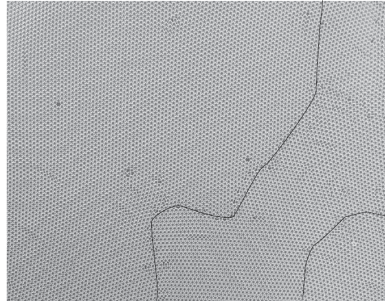


Figure 2: Grain boundaries in a bubble raft.

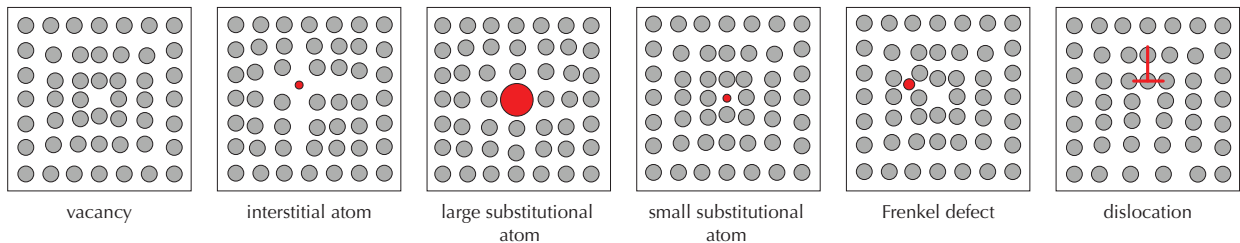


Figure 3: 2D defects in the square lattice.

Dislocations are topological defects, which makes them special and key ingredients of plastic deformation in crystalline materials. As already mentioned, their presence and dynamics crucially determine the material hardness. In fact, various techniques of working metals, including ancient crafts such as sword making, in significant part consist of achieving a certain organization of dislocations¹.

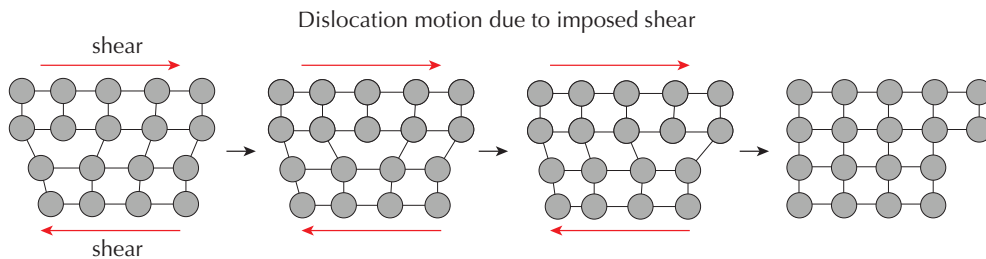


Figure 4: Dislocation propagation in the square lattice

Experimental setup

Material: You will use a plexiglas pool, a mixture of glycerin, water and surfactant, a small microfluidic device, syringe, syringe pump, plexiglas bars, small torch and a camera with a video option.

Fill the pool with the glycerol+water+surfactant mixture (unless it is already filled). Carefully place the microfluidic device into the round container that is located in one corner of the pool. Place the syringe into the pump holder and load it with air. Connect the microfluidic device with the syringe (see figure 5). Mount the camera, ensure it is stable, centered and horizontal.

¹NB: The main limitation of this bubble raft analogy is the two-dimensional nature of the raft. In reality bulk crystals are three-dimensional and have an entire class of screw dislocations which cannot exist in a two-dimensional bubble raft; all the dislocations we will see in the bubble raft are pure edge dislocations.

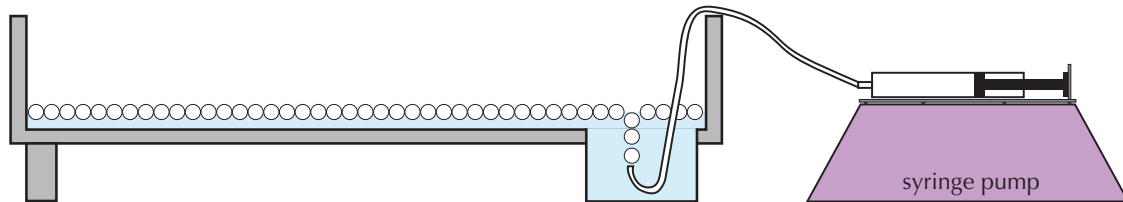


Figure 5: Experimental setup.

Part one *sur place*:

1) Set up the pump - injection speed should be $0.8\text{ml}/\text{min}$. This speed produces \sim millimeter bubbles. It will take you up to an hour (i.e., 2-3 loadings of the big syringe) to fill around a half of the pool. The bubbles should be relatively mono-disperse and forming a lattice. Above the microfluidic device a buildup of bubbles can be formed. From time to time you can either blow on the bubbles to move them or use the plexiglas bar to push them gently to the middle of the pool. If smaller or bigger bubbles form you can use blowtorch to pop the bubbles (carefully, though, as you can easily pop bubbles you would like to keep!)

As the raft is assembling, which may take up \sim 1hr, prepare for measurements by reading the “Concepts and Measurements” section below. As you think about the concepts, objects and behaviors described, observe your assembling raft and try to imagine or identify them.

- 2) Once the bubble raft is ready you will start photographing and filming with the camera and study:
- Grain boundaries
 - Vacancies
 - Dislocations and their dynamics (glide motion)
 - Recrystallization

The details can be found in “Concepts and Measurements” below. Make sure your photographs are of good quality and that your movies are focused and both capture different static and dynamic behavior as **you will be making a movie that contains your observations.**

- 3) Start a new recording on the camera. With this setup of the bubble raft you will study:
- Dislocation interactions
 - Annihilation of two dislocations

Concepts and Measurements

1) Make photos of your raft, close ups but also full field. The bubbles in the raft, just like atoms in a crystalline material, are mostly organized into a periodic arrangement, a lattice.

- Which lattice do you recognize in the raft?
- How many directions (axes) do you see along which the bubbles are most densely packed?
- These are analogous to crystal axes. Which angle do the axes (ideally) form?
- Does this lattice arrangement appear within three-dimensional crystals?

Instead of a single perfect lattice throughout the raft, you should see patches. These patches are analogous to **crystal grains** in polycrystals (see figure 2). Each patch has a lattice, but the axes are misaligned between a patch and a neighboring patch. The angle by which the axes are misaligned is **the mismatch angle**. Note that all axes on a given lattice are equivalent by symmetry.

- What is then the maximal angle of misalignment between grains?

The boundary line where the patches meet is a **grain boundary**. The grain boundary has two key properties: the mismatch angle across it, and the boundary line itself. The boundary line is approximately a straight line and forms a certain angle (the “boundary angle”) with respect to the axes of the two grains.

- Focus on one photo of the raft. Observe all patches and grain boundaries. Mark the grain boundaries and estimate the average diameter of each patch and record the size distribution of patches.
- Draw approximate straight lines for well-defined grain boundaries. Record the mismatch angle across each grain boundary. Record its boundary angle.
- Is there any regularity in the mismatch angles? How about the boundary angles?

2) Each patch is defined by a nice lattice of bubbles, but it is still not perfect. There should be a few point defects, like in figure 3.

- Pick images of the raft and mark examples of the following defects:
 - Substitutional impurity (one bubble of different size than other, sitting on a lattice site).
 - Vacancy (one bubble missing from a lattice site).
 - Interstitial (one bubble pushed in between other bubbles that would form a perfect lattice without it).
 - Look for combined defects, such as Frenkel defects (an interstitial and a vacancy near to each other).

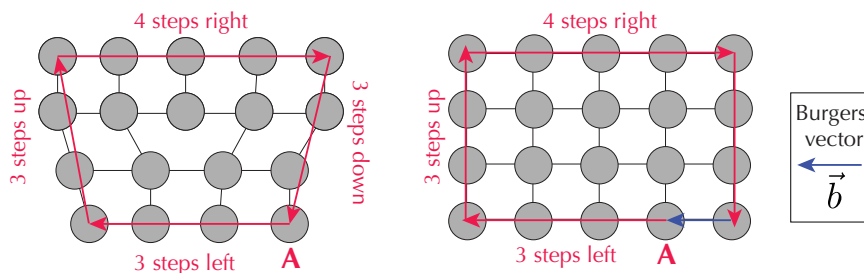


Figure 6: Constructing a burgers circuits. The Burgers vector \vec{b} is marked with a blue arrow.

- Identify dislocations - at a glance they may look like an ordinary point defect. You will identify them in two ways: a geometric way in a photo (like in figure 3), and a dynamical way (like in figure 4).
 - The dynamical identification of a dislocation is not rigorous, but it is simple way to find candidates. Gently push on the raft with a plexiglas bar. Some defects will rapidly move in a straight line along an axis when you do this, and these are (probably) dislocations. As you move back and forth, the defects should also move in reverse. Locate one of these defects near the centre of a grain, and perform the geometric identification described below.
 - The geometric identification rigorously proves that a defect is a dislocation, based on a topological property, the **Burgers vector**. To find this vector, which is zero for other point defects but has a characteristic non-zero value for a given dislocation, you must construct a **Burgers circuit** (see figure 6 with an example constructed for the square lattice).

Print a photo of the system. Choose a bubble a few rows away from the defect that you believe is a dislocation. Call this bubble A (see figure 6). Independently on a paper sketch a piece of a perfect lattice and mark a site corresponding to A. Now perform a clockwise circuit, jumping from one bubble to the next, starting and ending at bubble A; most importantly you must enclose the defect in your circuit. For each step in the circuit, mark the corresponding step on the perfect lattice. For example, to go back to A you might have to go 3 bubbles horizontally to the left, 5 up, 4 steps right, etc., and for each jump you must make the same axis and direction jump on the paper. However, the circuit that you have drawn on the paper might not end back at bubble A. This failure to close the circuit is the signature of a dislocation: if you have a point defect, such as a vacancy, there will

be no closure failure. For a clockwise circuit, mark the vector on paper from the finish site to the starting A site: **this is the Burgers vector**, and it must be a lattice vector, i.e., connecting two lattice sites. *The circuit needs to be big enough so that you are jumping on well-defined directions. Note that you can change the shape and size of the circuit but the resulting vector will remain the same — the Burgers vector is a topological property of a defect.*

- If you found a dislocation, record the piece of the video of its moving, and the photo with the marked Burgers circuit, and the corresponding circuit on paper.
- Now you should be able to identify the center of dislocation, and notice that it is located at a point where a line of closely-packed bubbles ends. Look along lines of bubbles starting from the center.

Is the extra line of bubbles uniquely defined?

Now notice that this part of the raft is divided into two halves by this center bubble: one half has an extra line of bubbles compared to the other.

Can you confirm that the Burgers vector is oriented along the division line of two halves?

- Go back to the video of the given dislocation. The movement you have seen happens along a line of bubbles.

Can you confirm that the movement line corresponds to the direction of the Burgers vector, like in the figure 4?

The Burgers vector defines the way a **slip** happens in the crystal. It enables the crystal to deform more easily under external force, which in typical metal crystals lowers the shear modulus by several orders of magnitude. The key to an easy deformation is the movement of the dislocation along its Burgers vector, which is called a **glide motion**. Imagine a piece of perfect lattice - the glide of the two halves would require a simultaneous movement of an infinite line of bubbles by their neighboring infinite line of bubbles.

- Repeat previous four steps to find at least two dislocations moving along two different axes.
- As you gently move the plexiglas bar back and forth, do you notice the same defects moving back and forth? Record the lattice axes directions (relative to the box) along which they move.
- Try to move dislocations further.

What happens when dislocations reach the edge of the raft, or a grain boundary?

You might even see two dislocations meeting each other - what happens? Do dislocations interact with point defects, such as vacancies, interstitials and substitutional point defects in the raft? If so, how? Describe. Try to record any such interaction (not easy!).

References

- [1] W. L. Bragg and J. F. Nye. A dynamical model of a crystal structure. 190, 1947.
- [2] G. I. Taylor. The mechanism of plastic deformation of crystals. part i. theoretical. *Proceedings of the Royal Society of London. Series A, Containing Papers of a Mathematical and Physical Character*, 145(855), 1934.
- [3] Vito Volterra. Sur l'équilibre des corps élastiques multiplément connexes. *Annales Scientifiques de l'École Normale Supérieure*, 24, 1907.

TP Bubble Raft - *à la maison*

You need to finish analyzing your data and make a movie that summarizes your observations.

Additionally, you will use numerical simulations and some analysis code to:

- Learn how two pair correlation functions look like for a crystal
- Understand how lattice defects influence the pair correlations
- Attempt to qualify the crystal nature of your bubble raft
- Study recrystallization of a bubble raft

Python code

There are two python-based programs that you can download from the TP HMP website, **BubbleRaft.ipynb** and **BubbleRaftJAX.ipynb** or you can find on the computer designated for this TP (the one you are using for the first part of the TP). If you have difficulty getting the files please let us know and we will send them to you via email.

Setup

To complete this TP you need to have either **python** installed together with an installation of the **Jupyter Notebook**, or you need to have a **gmail account**.

If you have a python installation on your computer it is easy to install a jupyter notebook. With miniconda you can use the following code in terminal:

```
conda install -c conda-forge jupyterlab
conda install -c conda-forge notebook
```

If you have pip installed please use the following code in terminal:

```
pip install jupyterlab
pip install notebook
```

Once this is done, in terminal go to the folder where you saved the notebooks and all the image files and simply type **jupyter notebook**. This command will launch in your web-browser the content of the folder you are in, and from there you can just click on the notebook you want to run.

If you don't have a python installation or if you simply don't have a good computer, please make a gmail account - it will take you 5 minutes. Once you have the account, you will have access to something called **google colab**, a web-based interface that allows you to run python jupyter notebooks on **google server** without needing to install anything on your computer. Additionally, you will get a **google drive**, space on google servers where you will need to copy the python notebooks for this TP as well as some of images you made in the lab, that you will be analyzing further.

For Google Colab users

Open your google drive by typing this in your browser www.drive.google.com. Once you login, you will first need to upload the notebooks and some of your images to the drive. Afterwards, navigate to the folder where you did this, locate the jupyter notebook you want to run and just select **Open with Google Colaboratory**, like in figure 7. This will open the notebook in colaboratory. You will need to mount your google drive as explained below, so you can have access to the images you need to use for the analysis.

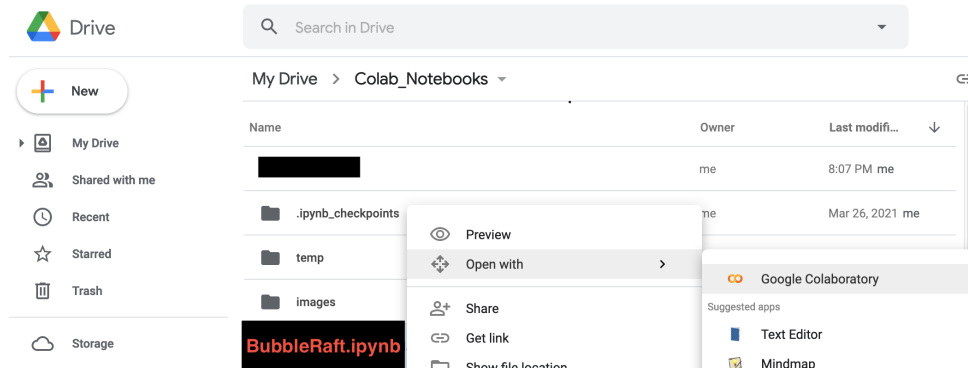


Figure 7: From google drive to colaboratory.

If you made your google account and have uploaded on your google drive the python notebooks, you can either open a desired notebook in the colaboratory or just visit the following webpage: <https://colab.research.google.com/notebooks/intro.ipynb>. You should see something like in the figure 8 below.

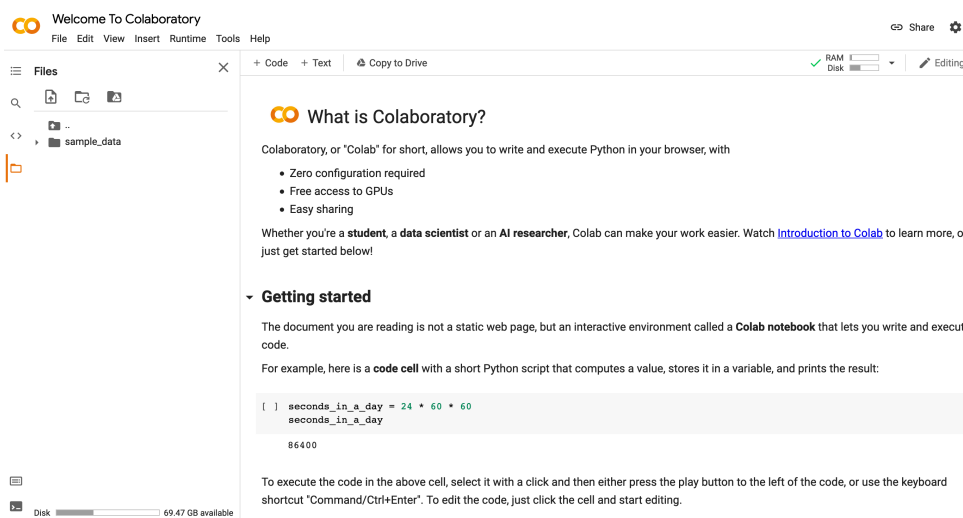


Figure 8: Google Colab intro page

The next step is to link the Colab with your google drive where all the notebooks and images are. You can do that by clicking on the drive icon (circled in the left in the figure 9 below). This will create a cell in the notebook that you need to run (click on the arrow that is circled in the right in the figure 9 below).

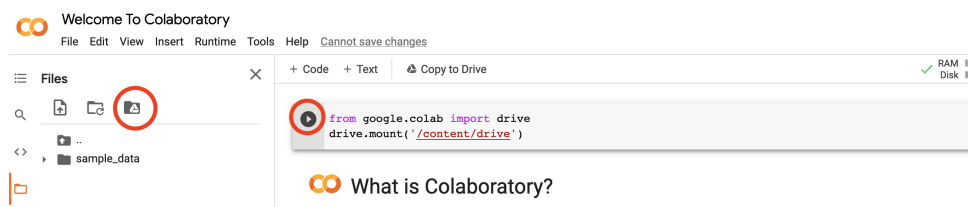


Figure 9: Mounting Google Drive

You will be shown an URL link that you need to follow. This will open a page asking you to allow linking between your drive and the colab and will subsequently give you an authorization code you need to paste in the cell marked with the second arrow in the figure 10.

Now that your drive is mounted, you can navigate to the folder where your notebooks and your data is, like in figure 11.

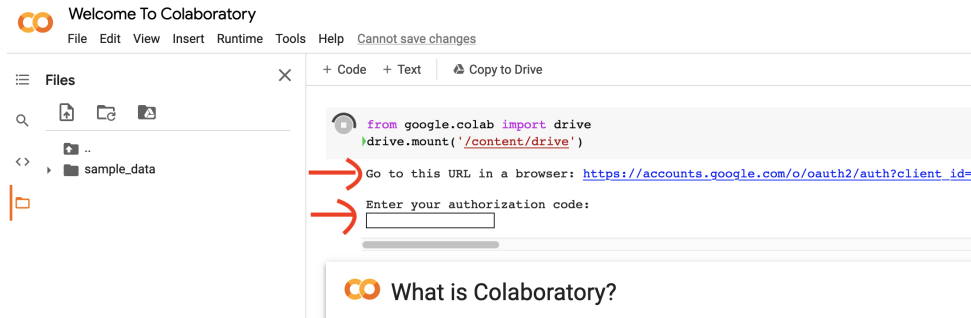


Figure 10: Final confirmation about linking your drive and colab.

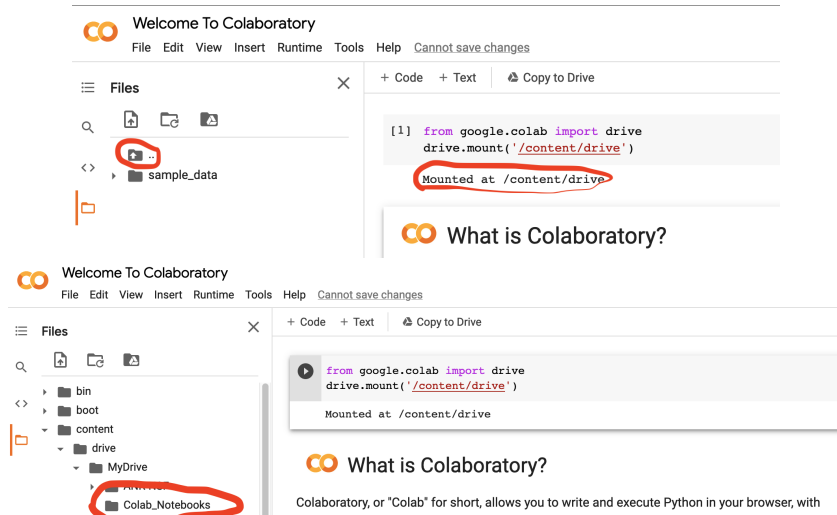


Figure 11: Navigate to the desired folder.

What will you do

You will continue to work on the bubble raft. First you will focus on how one can characterize the arrangement of bubbles in the raft, in particular the way it deviates from a perfect 2D crystal. For this you will use correlation functions, which you will apply to your images.

Concept: Correlation functions

A natural and useful way to characterize a spatial arrangement of N particles is through the Pair Correlation Function (PCF):

$$g(\vec{r}) = \sum_{i \neq j}^N \delta(\vec{r} - \vec{r}_{ij}), \quad (1)$$

where $\vec{r}_{ij} \equiv \vec{r}_i - \vec{r}_j$ is the relative vector of a particle pair, the δ is the Dirac delta function, so that the g measures the distribution of distance vectors in the system. If the particle positions \vec{r}_i form a perfect crystal, their relative positions also form a very precise set determined by the geometry of lattice, so that the $g(\vec{r})$ will have sharp peaks at a discrete set of values of \vec{r} . As the particles deviate from the perfect lattice positions due to elastic deformations but even more due to defects such as dislocations, grain boundaries, interstitials and others, the $g(\vec{r})$ becomes smoother with wide peaks. As the crystal becomes more disordered and eventually melts into a liquid, the g becomes flat and featureless for larger $|\vec{r}|$, i.e., the pair correlations are diminished: knowing position of one particle we cannot predict where any distant particle should be, the regularity in positions is lost.

The pair correlation function is measured quite directly in essential experiments of condensed matter physics! Some key experiments for studying material structure are elastic scattering experiments, in which some quantum particles (X-rays, neutrons, electrons) are shot at the material and then observed at the same energy but scattered by a vector \vec{q} . To illustrate the connection to g , one may assume weak scattering without absorption, where particles in the system are identical and isotropic. Then a particle at position \vec{r}_i creates a scattered plane-wave $b \exp(i\vec{q} \cdot \vec{r}_i)$, and the total scattered

wave is $\psi_q = b \sum_i^N \exp(i\vec{q} \cdot \vec{r}_i)$, so the scattered intensity measured in the experiment is:

$$I_q = \psi_q^* \psi_q = |b|^2 \sum_{i,j}^N \exp(i\vec{q} \cdot (\vec{r}_i - \vec{r}_j)). \quad (2)$$

One therefore defines the central quantity $S(\vec{q})$, the *static structure factor*, by:

$$S(\vec{q}) \equiv \frac{1}{N} \sum_{i,j}^N e^{i\vec{q} \cdot (\vec{r}_i - \vec{r}_j)} = 1 + \frac{1}{N} \int dV e^{i\vec{q} \cdot \vec{r}} g(\vec{r}), \quad (3)$$

where the connection to the pair correlation function is shown by simple use of the Dirac delta function. It turns out that the structure factor measured by scattering is given by the Fourier transform of the pair correlation function (note, the full technical definitions of these quantities differ slightly from this simplified description).

For simplicity, one correlation function we will focus on measures only the distances between particles, i.e., \vec{r}_{ij} is replaced by its length $|\vec{r}_{ij}|$ in the definition of g :

$$g_{\text{dist}}(r) = \sum_{i \neq j}^N \delta(r - |\vec{r}_{ij}|), \quad (4)$$

see for further details https://en.wikipedia.org/wiki/Radial_distribution_function.

The g_{dist} essentially measures whether a **translation** of a particle a certain distance away is likely to land on another particle. A complementary correlation function instead measures whether a **rotation** of a bond between particles by a certain angle lands on another bond. More precisely:

$$g_{\text{angle}}(r) = \left| \sum_{a,b}^{\text{NN pairs}} \delta(r - |\vec{R}_a - \vec{R}_b|) e^{6i(\theta_a - \theta_b)} \right|, \quad (5)$$

where $\vec{R}_a \equiv (\vec{r}_i + \vec{r}_j)/2$ is the center-of-mass of a nearest-neighbor pair of particles, the angle θ_a is the one formed by their link \vec{r}_{ij} with the global x-axis. In a perfect triangular lattice a particle has 6 nearest-neighbors, and the angles of these 6 links to some global axis are $\theta_0 + n \cdot 2\pi/6$, $n = 0, \dots, 5$, so that all links contribute identically to the exponent, namely $e^{6i\theta_0}$. As the lattice becomes imperfect, the correlation function $g_{\text{angle}}(r)$ measures the matching of the local rotation angles θ_0 between particles separated by a distance r .

The distinction between $g_{\text{dist}}(r)$ and $g_{\text{angle}}(r)$ is especially interesting in 2D, in which ordinary crystals have peculiar properties: at large length scales r the former correlation function decays as power-law because of disorder caused by occasional dislocation topological defects, while the latter correlation function is constant (local six-fold axes are oriented the same way in entire system). The proliferation of dislocation defects as temperature rises leads to *liquid-crystal* phases, in which the $g_{\text{dist}}(r)$ decays exponentially with r , while $g_{\text{angle}}(r)$ as power-law. At even higher temperatures other defects proliferate in the system and the crystal has melted into a liquid with all correlations decaying exponentially quickly.

Note that the definitions and explanations above are also contained in the python notebooks you will be using.

The BubbleRaft.ipynb notebook

You will start by loading images of your bubble raft: at least two images, one with many grains and defects, and one with as few as possible. You will also generate an image of a perfect triangular lattice to act as a reference perfect crystal. Using these images you will:

- Learn how two pair correlation functions look like for a crystal
- Understand how lattice defects influence the pair correlations
- Attempt to qualify the crystal nature of your bubble raft

The BubbleRaftJAX.ipynb notebook

You will start by generating a system of particles, and letting it relax to the lowest energy state using MD simulation. You will also relax the system after mixing up the particles (to "simulate" recrystallization). In these processes you will:

- Observe the most favorable lattice formed by particles in 2D
- Explore the presence of lattice defects, and their evolution during system relaxation
- Employ pair correlation functions to characterize the relaxed system