Experiment 4 Crystal and Reciprocal space

Objective

1. Demonstrating a fundamental understanding of crystals and the ability to describe the crystal structure.

2. Demonstrating a fundamental understanding of reciprocal space is the Fourier space associated with the crystal.
3. Basic understanding that the reciprocal lattice points can be mapped out by the set of reciprocal lattice vectors that yield planes waves with the periodicity of a given Bravais lattice.

Assignment Reading: https://www.youtube.com/watch?v=TicR6dcXSg0

Preparatory Questions

1. Define a crystal and provide its definition.
2. Explain the Fourier transform using a square pulse as an example. **Bonus**: Illustrate the Fast Fourier Transform (FFT) of a square pulse using Python.
3. Describe translation symmetry in physics and provide an example.
4. Identify the shapes (triangle, square, rectangle, parallelogram, rhombus, pentagon, hexagon, and octagon) that can completely cover a space through translation operations without gaps or overlaps.
5. What are diffraction and interference? Please look up the diffraction pattern of single-slit experiment. Does this diffraction pattern appear similar to the result you obtained from question 2?

Introduction

A crystal is a solid material whose atoms, or molecules are arranged in an ordered and repeating pattern, leading to distinctive properties and behaviors. Describing a crystal in a mathematical way involves defining its structure in terms of a lattice (point) and a basis. Here's an overview of how this is done:

- **Lattice (point):** A lattice is a repetitive arrangement of points in a vector space.

Lattices that exhibit a discrete translational symmetry are called Bravais lattices. For the bulk three-dimensional (3D) crystal, the Bravais lattice is defined by three fundamental translation vectors or primitive lattice vectors $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$. These vectors are chosen in a way that the atomic arrangement of the crystal appears identical after translation operation. Translation vector $\vec{T}$ is given by:

$$\vec{T} = n\,\mathbf{a_1} + m\,\mathbf{a_2} + l\,\mathbf{a_3} \qquad (1)$$

where n, m, and l are integers and $\mathbf{a_1}$, $\mathbf{a_2}$, $\mathbf{a_3}$ are lattice vectors.

In a Bravais lattice, all lattice points are equivalent, meaning that all properties remain unchanged under translations by any vector. Additionally, an observer situated at one specific lattice point would perceive the same environment as if situated at any other lattice point.

- **Basis:** The basis represents the arrangement of atoms or groups of atoms associated with each lattice (point).

One can proceed to substitute the lattice points with more intricate entities known as the basis, such as a group of atoms, a molecule, and so on. This process results in the formation of a structure commonly known as a crystal (**Figure 1**).

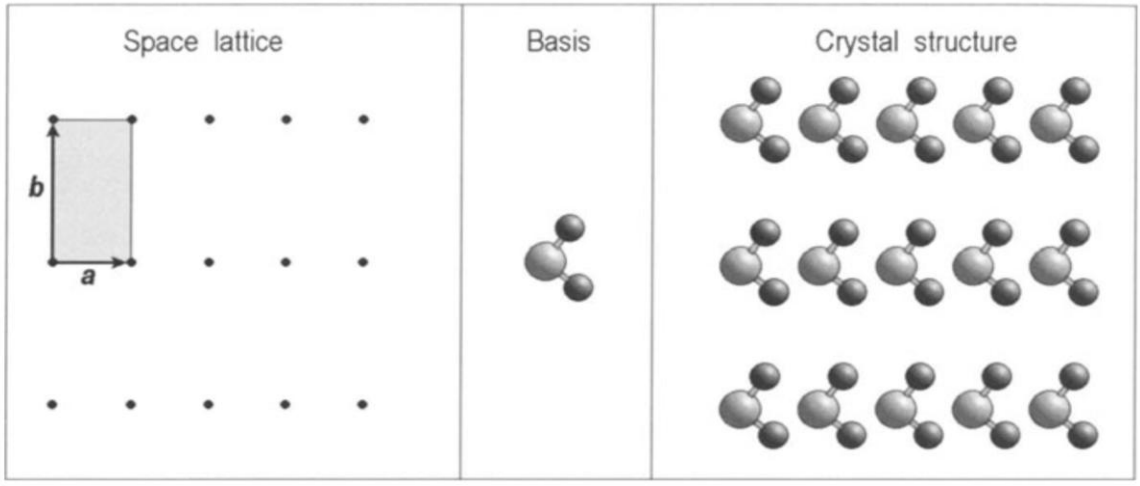
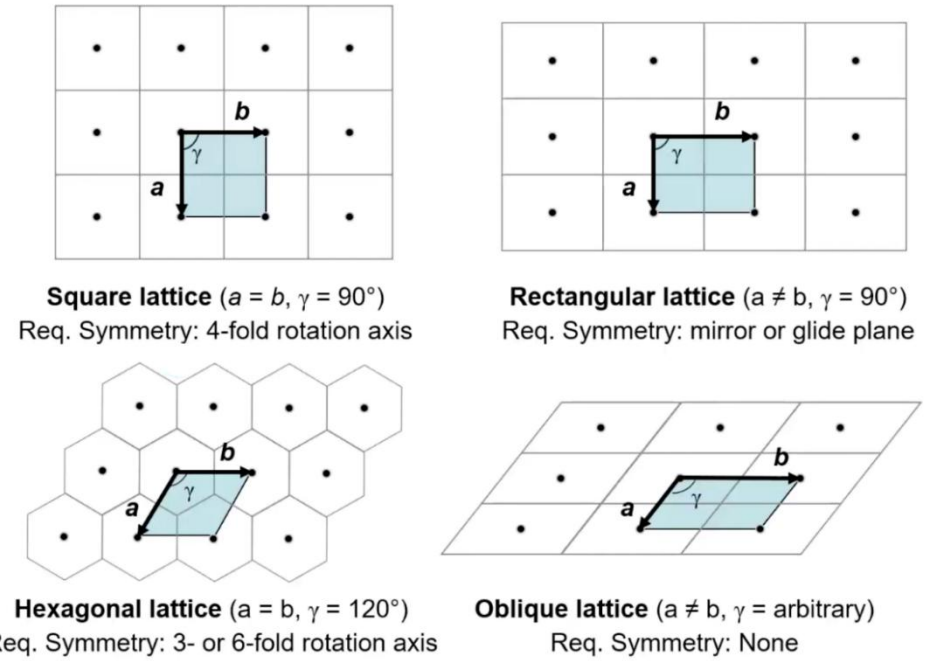


Figure 1. The crystal structure is formed by the addition of the basis to every point of the space lattice. [1]

In **Figure 1**, the geometric shape with sides **a** and **b**, forming a parallelogram, is referred to as a unit cell.

- **Unit Cell**: The unit cell is the repeating structure in a crystal that, when repeated in all directions through pure translation, reproduces the entire crystal without any overlaps or gaps.
- **Primitive cell**: A primitive cell is the smallest unit cell that encompasses precisely one lattice point. If a lattice point resides on the cell's edge, shared with another cell, it is counted as half.

Next, our focus shifts to the symmetry of crystals, illustrating the concept through two-dimensional (2D) crystals and their unit cells. We pose the question: which unit cell shapes (triangle, square, rectangle, parallelogram, rhombus, pentagon, hexagon, and octagon) can seamlessly tile space through translation operations, avoiding gaps and overlaps? This inquiry elucidates why only 2-fold, 3-fold, 4-fold, and 6-fold axes are viable



in 2D crystal [1]. Additionally, it pertains to the types of unit cells present in 2D crystals. **Figure 2** depicts the various types of unit cells in the 2D case.

Figure 2 type of unit cells of 2D crystal [2].

Exercise: Graphene Crystal Structure

Graphene is a single layer of carbon atoms arranged in a hexagonal lattice (**Figure 3**). In this exercise, we will explore the crystal structure of graphene and apply the concepts of lattice, basis, and lattice vectors.

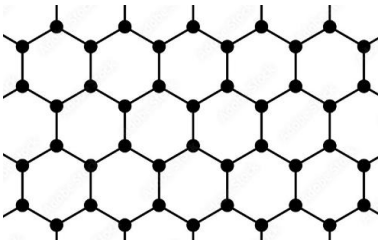


Figure 3 graphene crystal. Black dots represent the carbon atoms.

Exercise Questions

1.Describe the type of lattice present in graphene.

2. Identify the basis atoms in the unit cell of graphene.

3. How many carbon atoms constitute the basis?

4. Express the lattice vectors

5. Use these vectors to generate graphene lattice via python.

Bonus: 1. Use MATLAB/Python to create a twisted bilayer graphene Moiré pattern (in real space). 2. Find the relationship between periodicity of Moiré pattern and its twist angles.

Reciprocal Space

In this section, we turn to introduce reciprocal space. Reciprocal space, a fundamental concept in condensed matter physics, is analogous to the relationship between the time and frequency domains in signal processing. The Fourier Transform is employed to break down any signal into a combination of elementary sine and cosine waves, facilitating straightforward measurement of frequency, amplitude, and phase, as shown in **Figure 4**. []

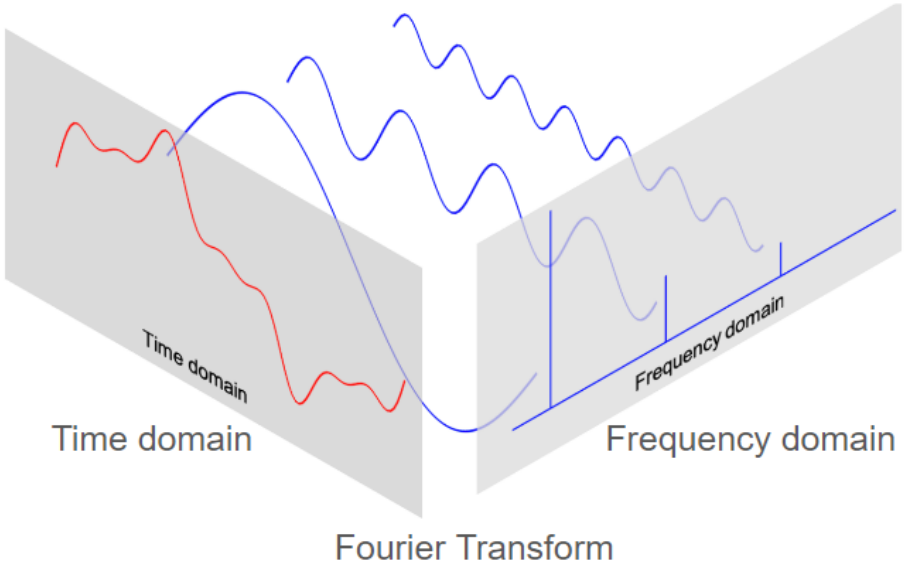


Figure 4 A complex signal expressed in both time and frequency domains [3]

In real space, the arrangement of atoms in a crystal is described by spatial coordinates, much like time-domain signals are represented by their amplitude variations

over time. The Fourier transform allows us to move seamlessly between these domains. Similarly, reciprocal space acts as the frequency domain counterpart, offering a unique perspective on the periodic structures found in crystals.

In the advanced experiments sections, we will learn why physicists find reciprocal space indispensable, particularly in the context of band structure studies. The band structure, a key aspect of condensed matter physics, illustrates how electrons move through a crystal lattice, influencing the material's electrical and optical properties.

In crystallography, the relationship between lattice vectors in real space and reciprocal lattice vectors in reciprocal space is described through the concept of the Fourier transform.

Reciprocal lattice:

The reciprocal lattice is defined as the set of all wave vectors that yield plane waves with the periodicity of a given Bravais lattice, as shown in **Figure 5** (parallel orange lines). Let **R** denotes a Bravais lattice point (**Figure 5**, black dots); consider a plane wave $\exp(i\mathbf{k}\cdot\mathbf{r})$ (**Figure5**, parallel orange lines). This will have the periodicity of the lattice if the wave vector **k** = **G**, such that $\exp(i\mathbf{G}\cdot(\mathbf{r}+\mathbf{R})) = \exp(i\mathbf{G}\cdot\mathbf{r})$ for any r and all **R** Bravais lattice. Thus, the reciprocal lattice vectors **G** must satisfy $\exp(i\mathbf{G}\cdot\mathbf{R}) = 1$. Therefore, $\mathbf{G}\cdot\mathbf{R} = 2\pi n$, where n is integer.

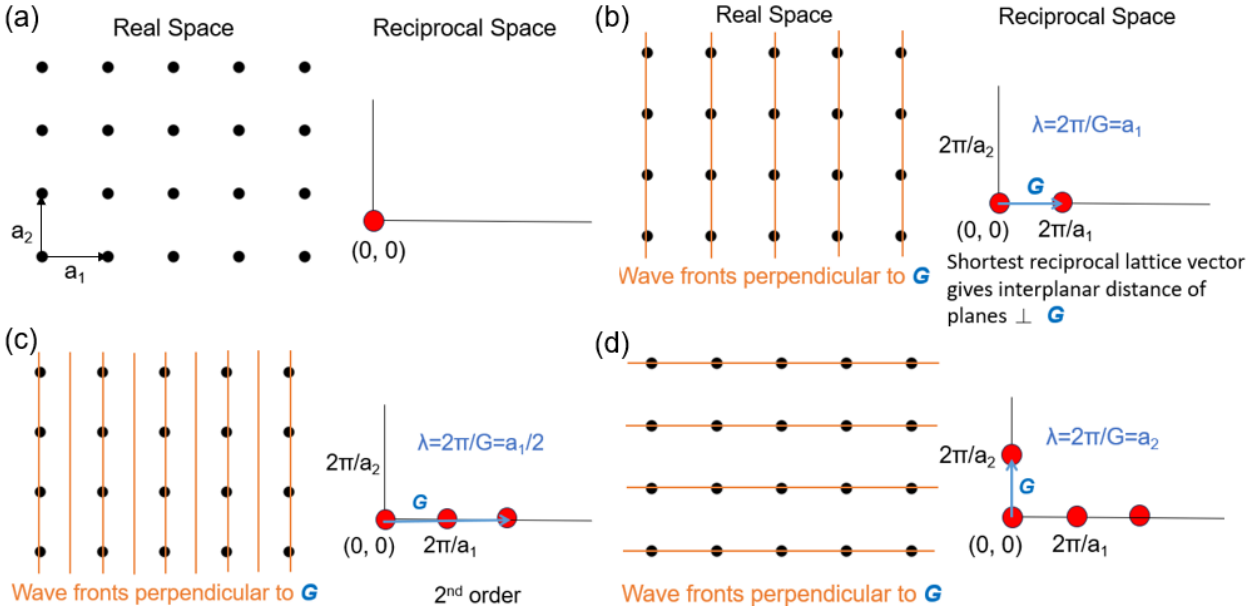


Figure 5 all reciprocal lattice vectors **G** that yield planes waves with the periodicity of a given Bravais lattice.

Let's summarize what we have discussed. If $\mathbf{a_1}$, $\mathbf{a_2}$, $\mathbf{a_3}$ are primitive lattice vectors, then $\mathbf{b_1}$, $\mathbf{b_2}$, $\mathbf{b_3}$ are primitive lattice vectors in reciprocal space. The reciprocal lattice vectors are defined as:

$$\boldsymbol{b_1} = 2\pi \frac{a_2 \times a_3}{a_1 \cdot (a_2 \times a_3)} \quad (3),$$

$$\boldsymbol{b_2} = 2\pi \frac{a_3 \times a_3}{a_1 \cdot (a_2 \times a_3)} \quad (4),$$

$$\boldsymbol{b_3} = 2\pi \frac{a_2 \times a_3}{a_1 \cdot (a_2 \times a_3)} \quad (5),$$

$$\mathbf{b_i} \cdot \mathbf{a_j} = 2\pi\delta_{ij} \text{ where } \delta_{ij} = 1 \text{ if } i = j \text{ and } \delta_{ij} = 0 \text{ if } i \neq j$$

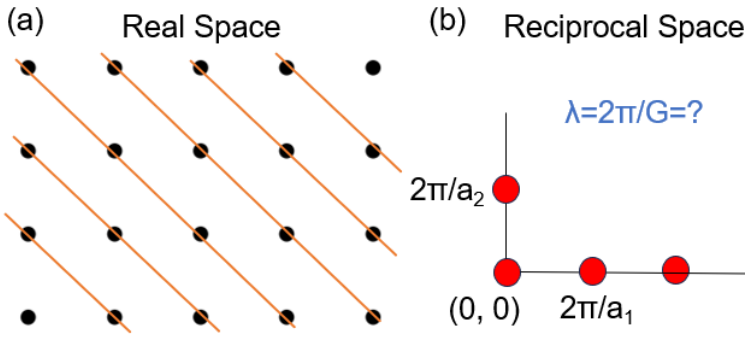
Points in the reciprocal lattice are mapped by the set of vectors

$$\mathbf{G} = v_1\mathbf{b_1} + v_2\mathbf{b_2} + v_3\mathbf{b_3} \quad (6),$$

where v_1, v_2, and v_3 are integers.

Exercise Questions

1. Pleas draw the reciprocal lattice vector G in Figure (b) and define the length of G.



2. Use this relationship ($\mathbf{b_i} \cdot \mathbf{a_j} = 2\pi\delta_{ij}$ where $\delta_{ij} = 1$ if $i = j$ and $\delta_{ij} = 0$ if $i \neq j$) to obtain the reciprocal lattice vectors of graphene and again use python to generate the reciprocal lattice point of graphene. Find the diffraction patterns of graphene from website and define the reciprocal lattice vectors. Compare these obtain vectors with your results.
3. Use the lattice points and the reciprocal lattice vectors you obtained from python to check if reciprocal lattice points can be mapped out by the set of reciprocal lattice vectors that yield planes waves with the periodicity of a given Bravais lattice (**Figure 5**).

Reference

1. Gross, D.J., *The role of symmetry in fundamental physics.* Proceedings of the National Academy of Sciences, 1996. **93**(25): p.14256-14259.

2. Diffraction Lecture 1: Translational Symmetry in Two Dimensions - YouTube

3. https://pythonnumericalmethods.berkeley.edu/notebooks/chapter24.02-Discrete-Fourier-Transform.html