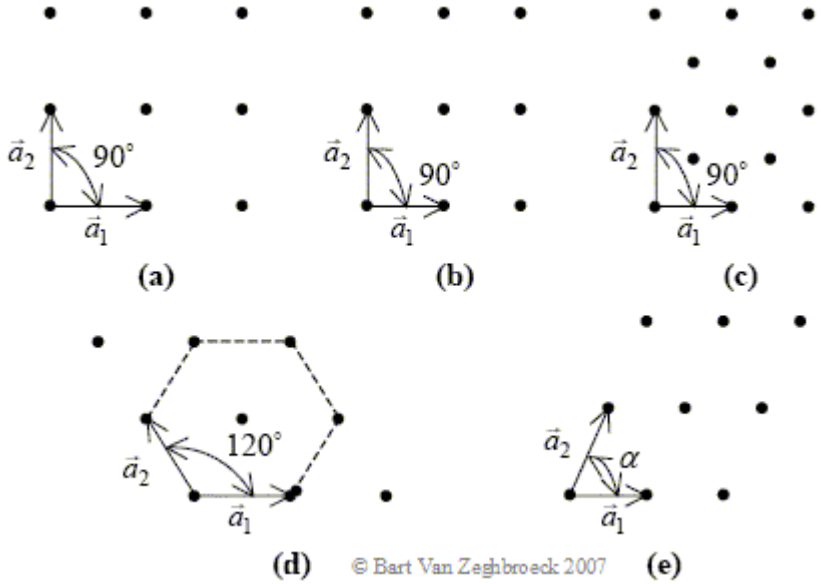
Lecture notes 3

HW 1 posted
Check that TA office hrs (Thurs 10-11am) work
Review key points of previous lectures:

- Primitive translation vectors



In a primitive lattice, every point can be accessed by:
-2 translation vectors in 2D: $\boldsymbol{T} = u_1\boldsymbol{a_1} + u_2\boldsymbol{a_2}$

-3 translation vectors in 3D: $= u_1\boldsymbol{a_1} + u_2\boldsymbol{a_2} + u_3\boldsymbol{a_3}$

Where $u_{1,2,3}$ are integers

Roadmap: Define reciprocal lattice and practice using it→some physical intuition for reciprocal lattice→Application of reciprocal lattice: formalism for understanding diffraction beyond Bragg's law→Making this formalism useful for all materials: using structure factor to account for diffraction from lattice + basis

Definition of reciprocal lattice vectors

The primitive translation vectors $\boldsymbol{a_1}, \boldsymbol{a_2}, \boldsymbol{a_3}$ represent the direct lattice.

The reciprocal lattice vectors, $\boldsymbol{b_1}, \boldsymbol{b_2}, \boldsymbol{b_3}$, are defined as follows:

$$\boldsymbol{b_1} = 2\pi \frac{\boldsymbol{a_2} \times \boldsymbol{a_3}}{\boldsymbol{a_1} \cdot \boldsymbol{a_2} \times \boldsymbol{a_3}}$$

$$\boldsymbol{b_2} = 2\pi \frac{\boldsymbol{a_3} \times \boldsymbol{a_1}}{\boldsymbol{a_1} \cdot \boldsymbol{a_2} \times \boldsymbol{a_3}}$$

$$\boldsymbol{b_3} = 2\pi \frac{\boldsymbol{a_1} \times \boldsymbol{a_2}}{\boldsymbol{a_1} \cdot \boldsymbol{a_2} \times \boldsymbol{a_3}}$$

- The denominator of all three is a scalar which gives the **volume** of the primitive cell: $V_c = |\boldsymbol{a_1} \cdot \boldsymbol{a_2} \times \boldsymbol{a_3}|$
- If a primitive lattice vector is mutually orthogonal to the other two, its reciprocal lattice vector will point in the same direction. If all three primitive lattice vectors of the direct lattice are mutually orthogonal, the reciprocal lattice vectors will all point in the same direction as the direct lattice vectors.
  if $\boldsymbol{a_i} \cdot \mathbf{a_j} = \delta_{i,j}$ for both values of j, $\boldsymbol{a_i} || \boldsymbol{b_i}$
- If primitive lattice vectors are all mutually orthogonal, the reciprocal lattice vectors point in the same direction at the direct lattice vectors but have a magnitude $2\pi/|\boldsymbol{a_i}|$
- Generalization of the previous two statements: $\boxed{\boldsymbol{b_i} \cdot \boldsymbol{a_j} = 2\pi\delta_{i,j}}$ where $\delta_{i,j} = 1$ if *i=j* and $\delta_{i,j} = 0$ if $i \neq j$

Example 1: orthorhombic lattice system

An **orthorhombic** lattice is comprised of rectangular prism cells with all edges of unequal length. The direct lattice vectors are:

$$\boldsymbol{a_1} = a\hat{\boldsymbol{x}}$$

$$\boldsymbol{a_2} = b\hat{\boldsymbol{y}}$$

$$\boldsymbol{a_3} = c\hat{\boldsymbol{z}}$$

Where $a \neq b \neq c$

- $\boldsymbol{a_1} \cdot \boldsymbol{a_2} \times \boldsymbol{a_3} = abc$
- $\boldsymbol{a_2} \times \boldsymbol{a_3} = bc\hat{\boldsymbol{x}}$
- $\boldsymbol{a_3} \times \boldsymbol{a_1} = ac\hat{\boldsymbol{y}}$
- $\boldsymbol{a_1} \times \boldsymbol{a_2} = ab\hat{\boldsymbol{z}}$

$$\boldsymbol{b_1} = \frac{2\pi}{a}\hat{\boldsymbol{x}}$$

$$\boldsymbol{b_2} = \frac{2\pi}{b}\hat{\boldsymbol{y}}$$

$$\boldsymbol{b_3} = \frac{2\pi}{c}\hat{\boldsymbol{z}}$$

For cubic, tetragonal, and orthorhombic primitive lattices, reciprocal lattice vectors are straightforward to compute—they are in the same direction as the corresponding direct lattice vector with a magnitude given by $2\pi/|\boldsymbol{a_i}|$. This is not true for crystal lattice systems in which the primitive lattices are not mutually orthogonal.

Example 2: Body-centered cubic

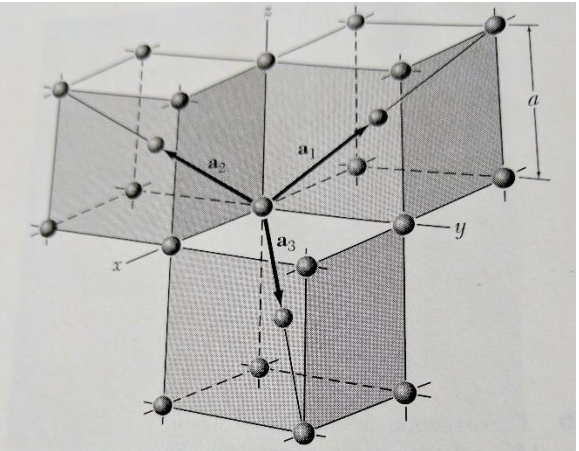


Figure 12 Primitive basis vectors of the body-centered cubic lattice.

The primitive lattice vectors of a BCC crystal system are shown by the arrows in this figure from your textbook. They consist of three vectors emanating from the corner of the unit cell and going to the body-center position in three adjacent cells (one can also write an equivalent vector starting at the body-centered position and going to three corners of the same cell). Using the definitions of the x,y,z directions from this figure (note: if you define x,y,z to be different directions, the vectors you wind up with won't be exactly the same as below, but they will be equivalent; always show what you define as x,y,z in you HW and exams), the expressions for these primitive vectors are:

$$\boldsymbol{a_1} = \frac{a}{2}(-\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}} + \hat{\boldsymbol{z}})$$

$$\boldsymbol{a_2} = \frac{a}{2}(\hat{\boldsymbol{x}} - \hat{\boldsymbol{y}} + \hat{\boldsymbol{z}})$$

$$\boldsymbol{a_3} = \frac{a}{2}(\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}} - \hat{\boldsymbol{z}})$$

Question: are these three vectors orthogonal?
Answer: no; e.g. $\boldsymbol{a_1} \cdot \boldsymbol{a_2} = \frac{a}{2}(-1 - 1 + 1) = -a/2 \neq 0$

Now let's calculate the reciprocal lattice vectors.

Step 1: calculate denominator, which is common to all three reciprocal lattice vectors:

$$\boldsymbol{a_1} \cdot \boldsymbol{a_2} \times \boldsymbol{a_3}$$

$$\boldsymbol{a_2} \times \boldsymbol{a_3} = \frac{a^2}{4}\begin{vmatrix} \hat{\boldsymbol{x}} & \hat{\boldsymbol{y}} & \hat{\boldsymbol{z}} \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{vmatrix} = \frac{a^2}{4}[\hat{\boldsymbol{x}}(1-1) - \hat{\boldsymbol{y}}(-1-1) + \hat{\boldsymbol{z}}(1+1)] = \frac{a^2}{2}[\hat{\boldsymbol{y}} + \hat{\boldsymbol{z}}]$$

$$\boldsymbol{a_1} \cdot \boldsymbol{a_2} \times \boldsymbol{a_3} = \left(\frac{a}{2}(-\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}} + \hat{\boldsymbol{z}})\right) \cdot \left(\frac{a^2}{2}[\hat{\boldsymbol{y}} + \hat{\boldsymbol{z}}]\right) = \frac{a^3}{4}(0 + 1 + 1) = \boxed{\frac{1}{2}a^3}$$

Step 2: calculate the numerators for all three reciprocal lattice vectors:

$$\boldsymbol{b_1} \propto \boldsymbol{a_2} \times \boldsymbol{a_3} = \frac{a^2}{2}[\hat{\boldsymbol{y}} + \hat{\boldsymbol{z}}]$$

$$\boldsymbol{b_2} \propto \boldsymbol{a_3} \times \boldsymbol{a_1} = \frac{a^2}{4}\begin{vmatrix} \hat{\boldsymbol{x}} & \hat{\boldsymbol{y}} & \hat{\boldsymbol{z}} \\ 1 & 1 & -1 \\ -1 & 1 & 1 \end{vmatrix} = \frac{a^2}{4}[\hat{\boldsymbol{x}}(1+1) - \hat{\boldsymbol{y}}(1-1) + \hat{\boldsymbol{z}}(1+1)] = \frac{a^2}{2}[\hat{\boldsymbol{x}} + \hat{\boldsymbol{z}}]$$

$$\boldsymbol{b_3} \propto \boldsymbol{a_1} \times \boldsymbol{a_2} = \frac{a^2}{4}\begin{vmatrix} \hat{\boldsymbol{x}} & \hat{\boldsymbol{y}} & \hat{\boldsymbol{z}} \\ -1 & 1 & 1 \\ 1 & -1 & 1 \end{vmatrix} = \frac{a^2}{4}[\hat{\boldsymbol{x}}(1+1) - \hat{\boldsymbol{y}}(-1-1) + \hat{\boldsymbol{z}}(1-1)] = \frac{a^2}{2}[\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}}]$$

Step 3: put it all together

$$\boldsymbol{b_1} = 2\pi \cdot \frac{2}{a^3} \cdot \frac{a^2}{2}[\hat{\boldsymbol{y}} + \hat{\boldsymbol{z}}] = \frac{2\pi}{a}[\hat{\boldsymbol{y}} + \hat{\boldsymbol{z}}]$$

$$\boldsymbol{b_2} = 2\pi \cdot \frac{2}{a^3} \cdot \frac{a^2}{2}[\hat{\boldsymbol{x}} + \hat{\boldsymbol{z}}] = \frac{2\pi}{a}[\hat{\boldsymbol{x}} + \hat{\boldsymbol{z}}]$$

$$\boldsymbol{b_3} = 2\pi \cdot \frac{2}{a^3} \cdot \frac{a^2}{2}[\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}}] = \frac{2\pi}{a}[\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}}]$$

Step 4: check your answer. Make sure that $\boldsymbol{b_i} \cdot \boldsymbol{a_j} = 2\pi\delta_{i,j}$

(only i=1; j=1,2 is shown below)

$$\boldsymbol{b_1} \cdot \boldsymbol{a_1} = \frac{2\pi}{a}[\hat{\boldsymbol{y}} + \hat{\boldsymbol{z}}] \cdot \frac{a}{2}(-\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}} + \hat{\boldsymbol{z}}) = \pi(0+1+1) = 2\pi$$

$$\boldsymbol{b_2} \cdot \boldsymbol{a_1} = \frac{2\pi}{a}[\hat{\boldsymbol{x}} + \hat{\boldsymbol{z}}] \cdot \frac{a}{2}(-\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}} + \hat{\boldsymbol{z}}) = \pi(-1+0+1) = 0$$

The reciprocal lattice is also a lattice (and if the direct lattice is primitive, then so is the reciprocal), and points in reciprocal space are mapped out by the set of vectors:

$$\boldsymbol{G} = \nu_1\boldsymbol{b_1} + \nu_2\boldsymbol{b_2} + \nu_3\boldsymbol{b_3}$$

Where ν_1, ν_2, ν_3 are integers.

Reciprocal lattice and fourier series

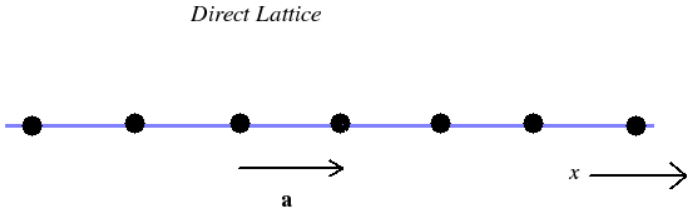
Now that we know what the reciprocal lattice vectors are, lets get some physical intuition behind them. A crystal is composed of infinitely repeating unit cells (unit cell = basis of one or more atoms attached to a lattice point). A crystal is invariant under translation of the form $\boldsymbol{T} = u_1\boldsymbol{a_1} + u_2\boldsymbol{a_2} + u_3\boldsymbol{a_3}$ where u_1, u_2, u_3 are integers and $\boldsymbol{a_1}, \boldsymbol{a_2}, \boldsymbol{a_3}$ are the lattice vectors. This is another way of saying that every unit cell is identical to every other unit cell. Although we have only been discussing nuclei thus far in the class, when we introduce electrons back into the picture, their arrangement and behavior will be directly affected by the underlying periodicity of the nuclei. The purpose of this chapter is to further develop the formalism for studying these infinitely periodic structures, and explore one of its most important applications—diffraction.

When we think of a periodic structure, whether it be a sine wave, a square wave, or some other more complicated shape which repeats with period a, we should immediately think of a fourier transform or a fourier series.

The example of Fourier transforms that we encounter most often in our everyday life is in music. We physically experience a given note in the **time** domain as an alternating compressions and decompression of the air near our ear, but we define a note by its **frequency** (e.g. 440 Hz). Similarly, we have been talking about the repetition of a crystal lattice in **real space**, but this redundancy is accounted for when we fourier transform to **momentum space** or(also known as) **reciprocal space.**

Let's consider the **lattice** (no basis), which mathematically is represented by a series of delta functions. In this portion of the lecture, I deviate from Kittel's presentation a bit, and will post a scan of another book (structure and Dynamics, but Martin T. Dove).

Only consider a one dimensional lattice at first, with spacing *a* between lattice points.



This structure can be written as: $L(x) = \sum_{u_1} \delta(x - u_1 a)$, where u1 is an integer

The Fourier transform of this is given by:

$$R(q) = \int_{-\infty}^{\infty} e^{iqx} L(x) dx$$

$$= \sum_{u_1} \int_{-\infty}^{\infty} e^{iqx} \delta(x - u_1 a) dx$$

Aside: generally, the FT of a delta function is given by $\int_{-\infty}^{\infty} e^{iqx} \delta(x - x_0) dx = e^{iqx_0}$

Also, the FT is often expressed with a factor of 2pi in the exponent, but we will account for that later

$$= \sum_{u_1} e^{iqu_1 a} = \sum_{u_1} \cos(qu_1 a) + isin(qu_1 a)$$

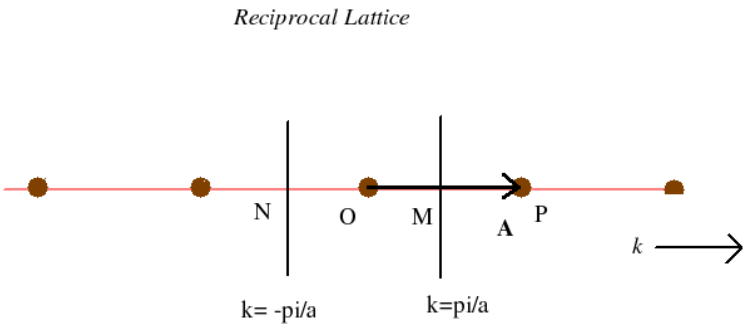
Simplification: we only need to keep the cosine term because the sum goes over positive and negative values of u1 and $\sin(-x) = -\sin(x)$

$$R(q) = \sum_{u_1} \cos(qu_1 a)$$

For arbitrary values of q, this sum will tend to zero as the number of terms goes to infinity. This can only be avoided if specific values of q are chosen:

$$q = \text{integer} \times \frac{2\pi}{a}$$

This gives a 1 dimensional lattice with points separated by $2\pi/a$. This is the reciprocal lattice.



This can be generalized to three dimensions:

$$L(\vec{\boldsymbol{r}}) = \sum_{u_1,u_2,u_3} \delta\big(\boldsymbol{r} - (u_1\boldsymbol{a_1} + u_2\boldsymbol{a_2} + u_3\boldsymbol{a_3})\big)$$

Where u_1, u_2, u_3 are integers and $\boldsymbol{a_1}, \boldsymbol{a_2}, \boldsymbol{a_3}$ are lattice vectors which span 3D space

Take the Fourier transform again same as in 1D:

$R(\boldsymbol{k}) = \sum_{u_1,u_2,u_3} cos\big(\boldsymbol{k} \cdot (u_1\boldsymbol{a_1} + u_2\boldsymbol{a_2} + u_1\boldsymbol{a_1})\big)$

Again, the sum will generally be non-zero only if **k** is a reciprocal lattice vector R(**k)**

$$\boldsymbol{k} = k_1\boldsymbol{b_1} + k_2\boldsymbol{b_2} + k_3\boldsymbol{b_3}$$

Thus, one physical interpretation of the reciprocal lattice is that it is the Fourier transform of the direct lattice, a mathematical operation which takes into account the repetition of the crystal lattice

2nd intuition: reciprocal lattice vectors as specific plane wave states

Consider a set of points **R** constituting a bravais lattice and a generic plane wave $e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$

For a general value of k, such a plane wave will not have the periodicity of the lattice, but for a certain choice of k, it will:

The set of all wavevectors **K** which yields plane waves with the periodicity of the lattice is known as the reciprocal lattice

The way to state this mathematically, is that the following expression applies for all spatial coordinates **r** (why? Because the **R** vector is defined as a translation operation which leaves the lattice invariant)**:**

$$e^{i\boldsymbol{K}\cdot(\boldsymbol{r}+\boldsymbol{R})} = e^{i\boldsymbol{K}\cdot\boldsymbol{r}}$$

$$e^{i\boldsymbol{K}\cdot\boldsymbol{R}} = 1$$

This expression holds if $\boldsymbol{K} \cdot \boldsymbol{R}$ is an integer multiple of 2π, which we showed in the exercise above