Some Notes On Lattice And Diffraction

Yuanpeng Zhang

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School of Physics and Astronomy

Queen Mary, University of London

In this article, several aspects about the understanding of lattice definition and the relationship with diffraction problem are discussed. It should be pointed out that the idea was not organized following exact logic, which, then, may seem to be a bit massy. However anyway, it should be somehow helpful for the understanding of lattice definition.

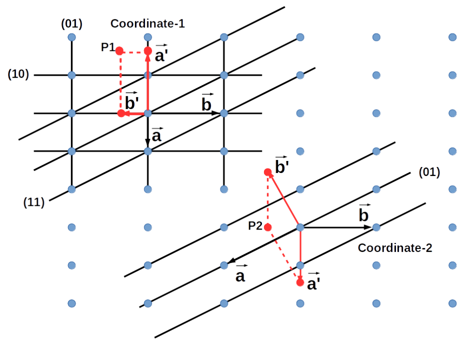

Figure 1: Example of a two-dimensional lattice structure.

Let's begin with a simple two-dimensional lattice structure as shown in Fig. 1. For the lattice shown in Fig. 1, when only considering the periodicity of the lattice, we can actually have several options for the coordinate system. Two typical instances are shown, which are labelled with Coordinate-1 and Coordinate-2, respectively. Once the coordinate system is pinned down, then all the lattice planes can be indexed, accordingly, as shown in Coordinate-1. Also the corresponding reciprocal space lattice points can be built up according to the basic rule for establishing reciprocal space. It should be pointed out that although different choice of coordinate system should definitely bring different index for the lattice plane and also different unit vector in reciprocal space, there is, in fact, nothing special for each coordinate system. Since the only difference between coordinates is indexing, however the periodicity does not depend on indexing, at all. For example, the 'P1' point (in reciprocal space) in Coordinate-1 is just the end of unit vector in Coordinate-2, and it is similar to the case of 'P2' point in Coordinate-2. Since the selection of coordinate system is arbitrary, to make life easier, Bravais defined several rules for the selection of unit cell, one of which is that there should be as many right angles, as possible, in the unit cell. Corresponding selected unit cell is called Bravais lattice. Therefore, obviously, the Coordinate-1 here in this case is our Bravais lattice.

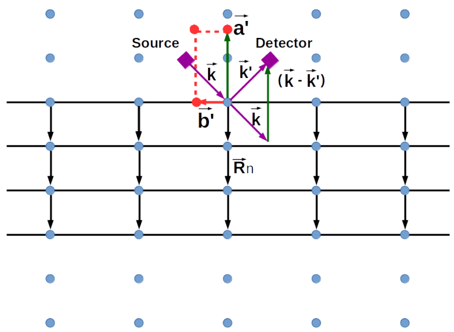

Figure 2: Diffraction in the example two-dimensional lattice.

In diffraction problem, what matters is the the phase difference between the outgoing and incoming beam (e.g. X-ray), and in the case shown in Fig. 2 it can be written down as $\Delta_{phase} = (\mathbf{k} - \mathbf{k}^{'}) \cdot \mathbf{R}_n$. As a result, the condition of diffraction maximum is just that the vector $\mathbf{k} - \mathbf{k}^{'}$ should be identical to one of the lattice vectors in reciprocal space, as shown in green-colour arrow in Fig. 2. So from this example, one can also get the idea that what diffraction experiment does is to transform the periodicity information in real space to its corresponding reciprocal space, i.e. doing the Fourier transform. Therefore the lattice point in reciprocal space actually represents the frequency components of the observed lattice (in real space).

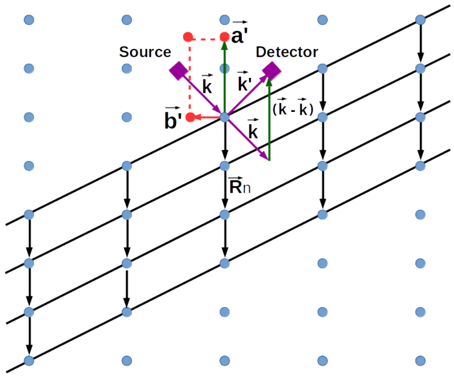

Figure 3: Diffraction in the example two-dimensional lattice, observing the periodicity from another perspective.

As discussed above, the diffraction experiment is actually observing the periodicity of the lattice. And here in Fig. 3, the periodicity is identical to that in Fig. 2, also the positions of the incoming beam source and the detector are kept the same as they are in Fig. 2. Therefore when calculating the phase difference following $\Delta_{phase} = (\mathbf{k} - \mathbf{k}^{'}) \cdot \mathbf{R}_n$, we could find that nothing changes as we change our observation angle for the periodicity. So for Fig. 2 and Fig. 3, we are actually observing the same thing!

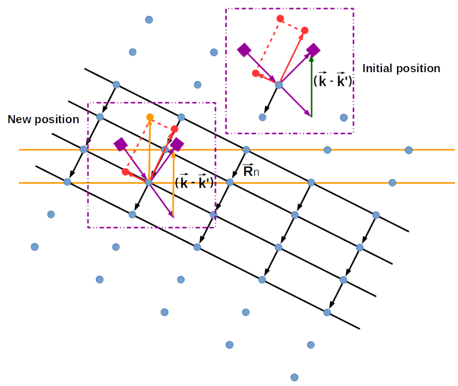

Figure 4: Diffraction in the example two-dimensional lattice. The lattice was rotated around an axis perpendicular to the paper, in this case.

Now, if keeping the source and detector not moving, meanwhile rotating the lattice to another position, as shown in Fig. 4, then considering the same periodicity as before ($\mathbf{R}_n$), we will not observe diffraction maximum. Why? First of all, the reciprocal space lattice point which $\mathbf{k} - \mathbf{k}^{'}$ falls onto in previous case (Fig. 2 & 3) has now rotated to a new position, in accordance with the rotation of real space lattice. So the same vector subtraction ($\mathbf{k} - \mathbf{k}^{'}$), in this case, misses the reciprocal space lattice point. From another perspective, the cross product $(\mathbf{k} - \mathbf{k}^{'}) \cdot \mathbf{R}_n$, becomes smaller, since in this case we have an angle between $\mathbf{k} - \mathbf{k}^{'}$ and $\mathbf{R}_n$, but not 0 (or 180) as it was before rotation.

Then how can we again get back the diffraction maximum in this case? Imagine decreasing the angle between the incoming (and also the outgoing) beam and the vertical line, the magnitude of $\mathbf{k} - \mathbf{k}^{'}$ will become larger than before. To some specific position, the cross product $(\mathbf{k} - \mathbf{k}^{'}) \cdot \mathbf{R}_n$ will again meet the condition of diffraction maximum, and again we will observe corresponding diffraction maximum. In another word, $\mathbf{k} - \mathbf{k}^{'}$, again, falls onto one of the lattice point in reciprocal space as shown by dark yellow colour in Fig. 4. Furthermore, it should be pointed out that, although we are again observing the same periodicity as before ($\mathbf{R}_n$), but in this case, the influence of the periodicity is different (remember the angle in the cross product due to the rotation of the lattice). Therefore, we have an equivalent periodicity, which corresponds to the lattice plane (11) as shown in dark-yellow-coloured line in Fig. 4.

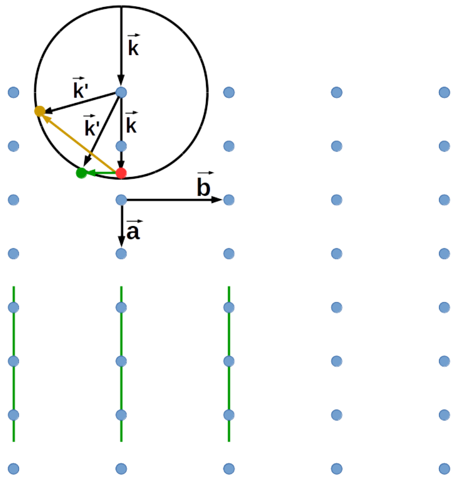

Figure 5: The illustration for the idea of Ewald 'circle' – the counterpart of Ewald sphere in two-dimension.

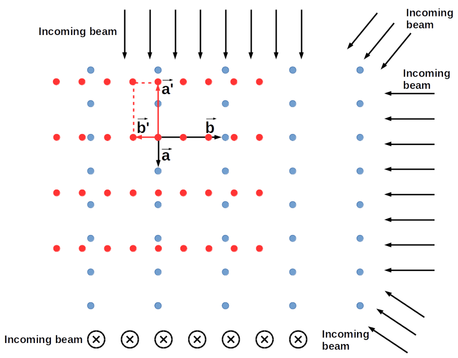

Figure 6: The building of full reciprocal space.

Now we may have the idea that to observer different equivalent lattice plane, we need to adjust the observation angle. Exactly speaking, we need to adjust $\mathbf{k} - \mathbf{k}^{'}$, which is in relation to both the wavelength and direction of incoming and outgoing detection beam. For elastic scattering problem, the wavelength does not change before and after the scattering, so actually we have two factors contributing to the phase difference (thus influence where we can observe the diffraction maximum) – angle and wavelength. As shown in Fig. 5, we now fix the direction of incoming beam with specific wavelength, and furthermore we set the origin of reciprocal space lattice at

the end of the incoming beam vector (the red dot shown in Fig. 5). Then if we continuously change the detection angle (which means if the starting point of the outgoing wave vector was fixed at the same point with that of incoming wave vector, it was then rotated continuously in a circle as shown in Fig. 5), in some specific conditions, we can observe diffraction maximum. What is the condition? As shown in Fig. 5, if the plotted circle happens to meet the lattice point in reciprocal space (the green and dark yellow colour points in Fig. 5), the vector $\mathbf{k}-\mathbf{k}^{'}$ then just falls onto corresponding lattice point in reciprocal space. Accordingly, we should observe the diffraction maximum. For example, when the circle in Fig. 5 meets the green point, the diffraction maximum corresponding to the green lattice plane in Fig. 5 will be observed. This is just the basic idea of Ewald 'circle', and in the case of 3D, it is called Ewald sphere.
Finally, as shown in Fig. 6, if changing the incoming beam direction freely, we could then build up the full reciprocal space lattice following the idea of Ewald 'circle'.