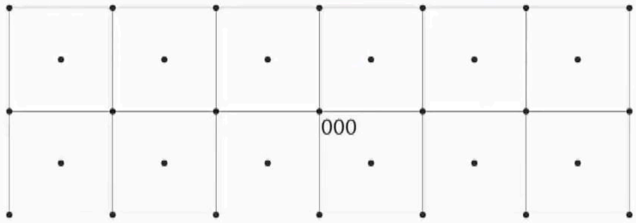
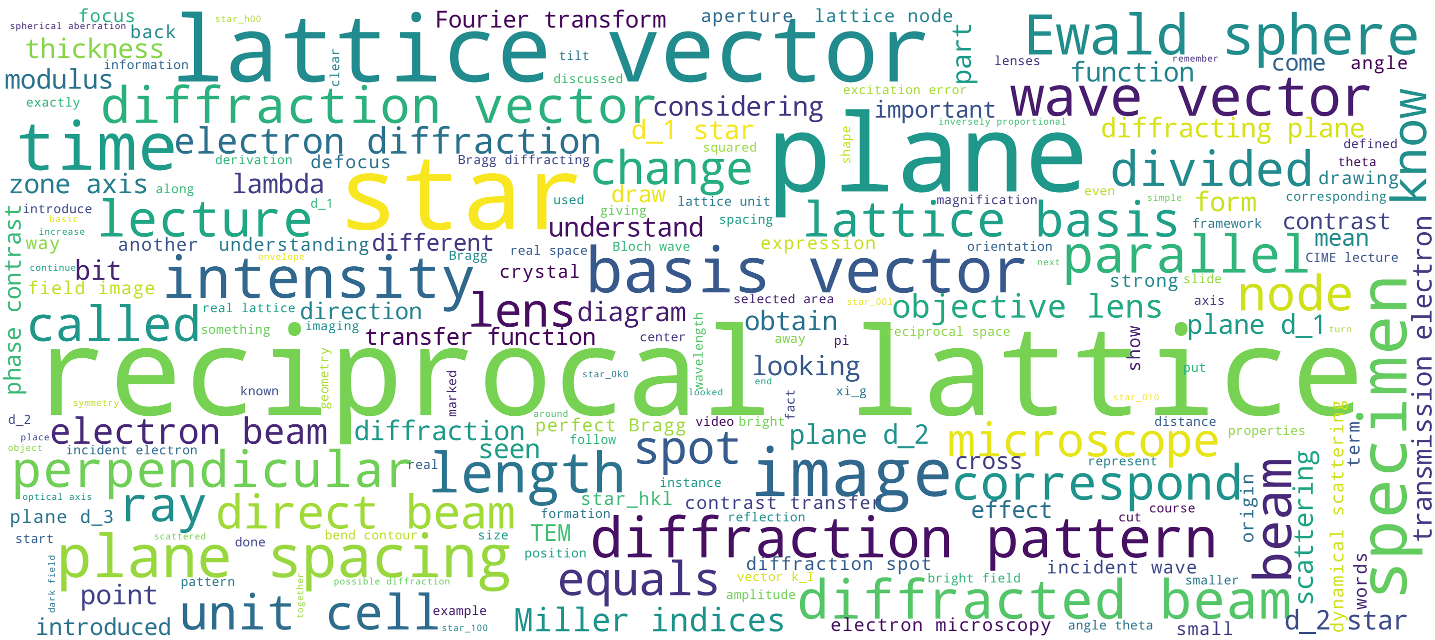
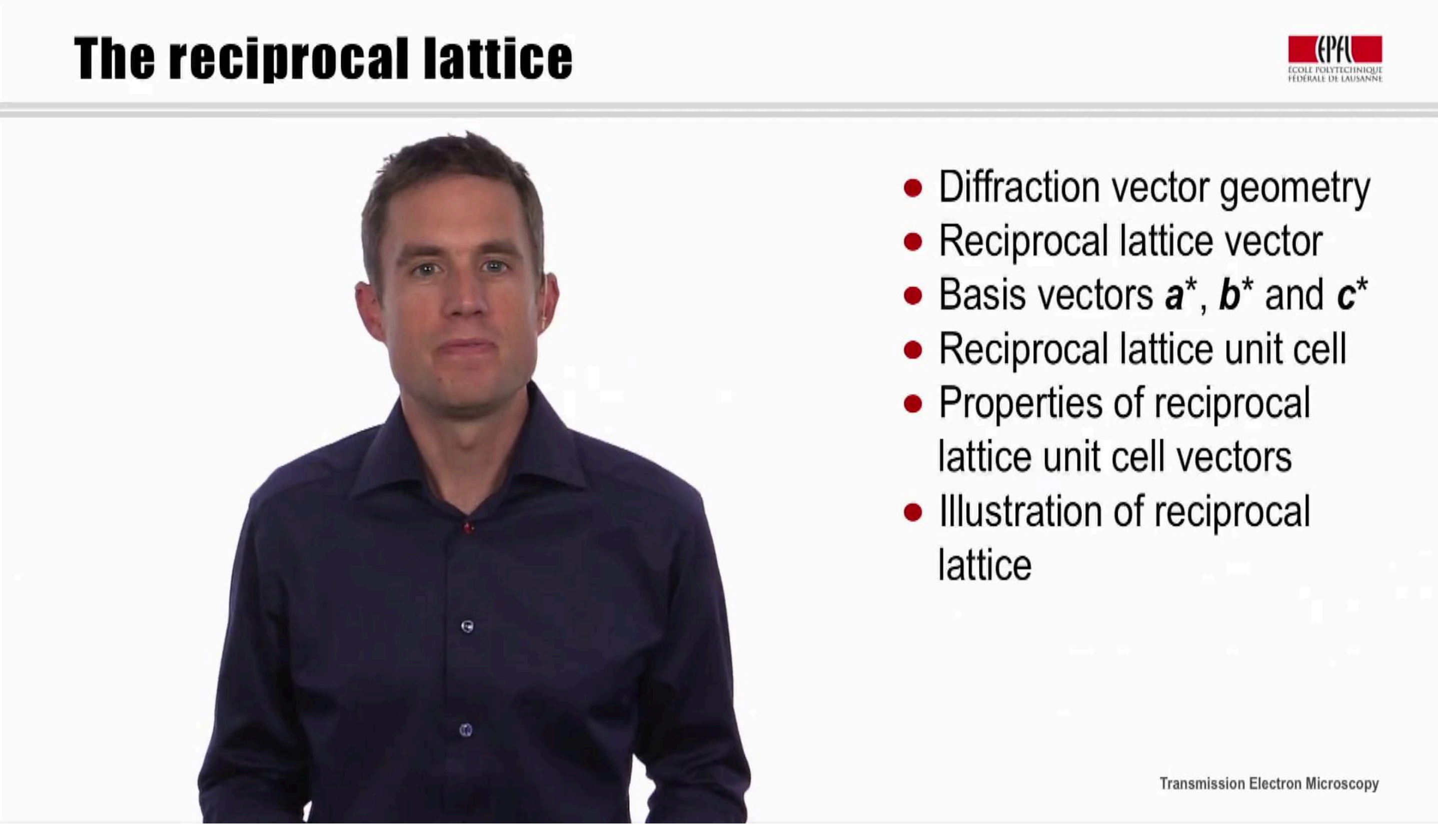


Basics of electron diffraction: reciprocal lattice

Transmission Electron Microscopy

Prof. C. Hébert & Dr D. Alexander



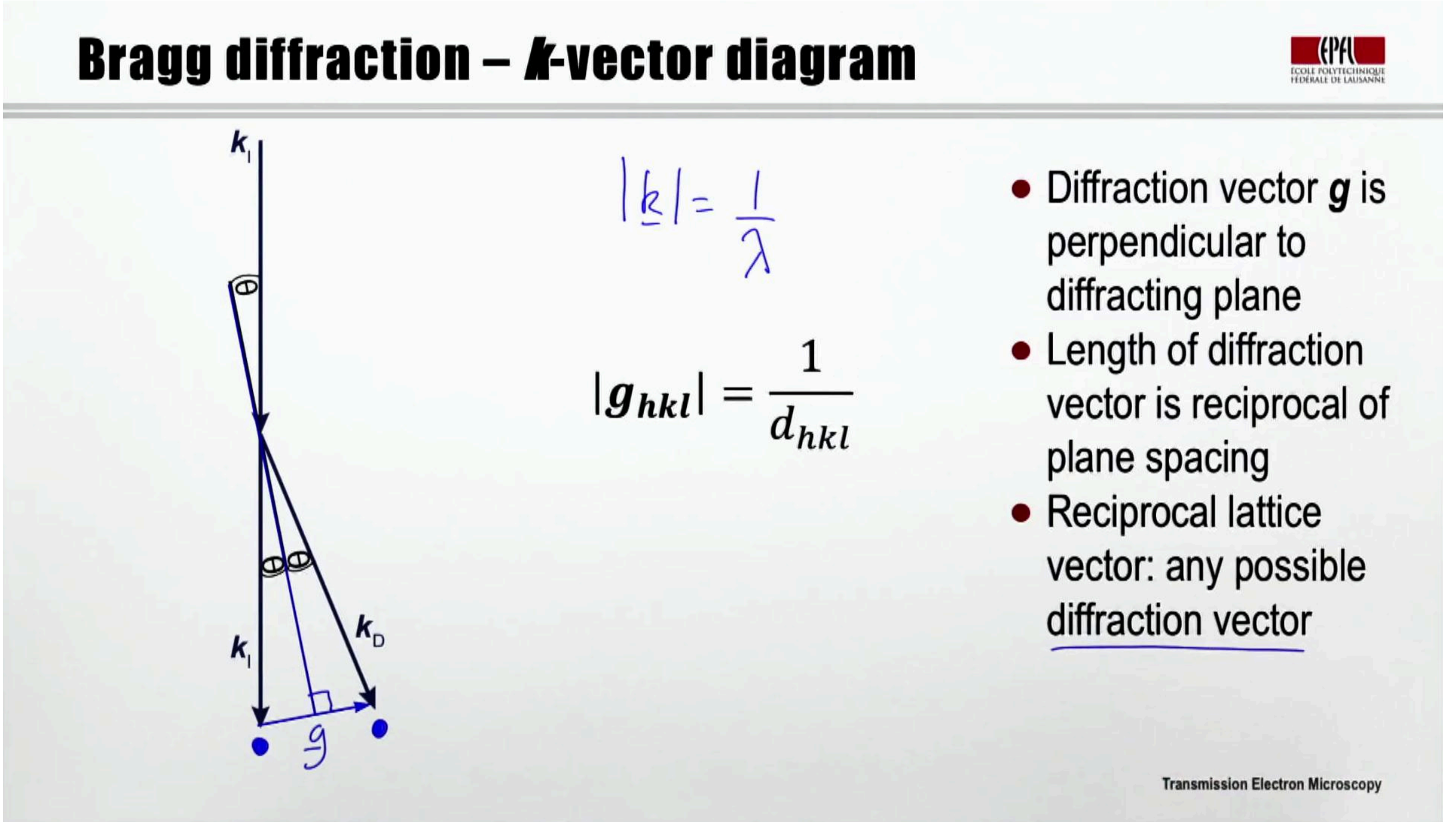


Welcome to CIME's lectures on transmission electron microscopy for materials science. Continuing on the theme of the basics of electron diffraction, in this lecture I will introduce the reciprocal lattice, which, together with the Ewald sphere, will form our framework for understanding and interpreting electron diffraction in the lectures to come. To consider the reciprocal lattice, I'm going to begin by considering the geometry of the diffraction vector, that was introduced last time. From there, I'm going to go on and look at reciprocal lattice vectors, and then the basis vectors of the reciprocal lattice: a-star, b-star and c-star. These form the reciprocal lattice unit cell, and have certain properties which will be discussed briefly. Then finally, I'm going to go from there, to looking at an illustrative schematic of a reciprocal lattice, which will then take further in the next lecture on the Ewald sphere.

Notes

Summary

0m 05s

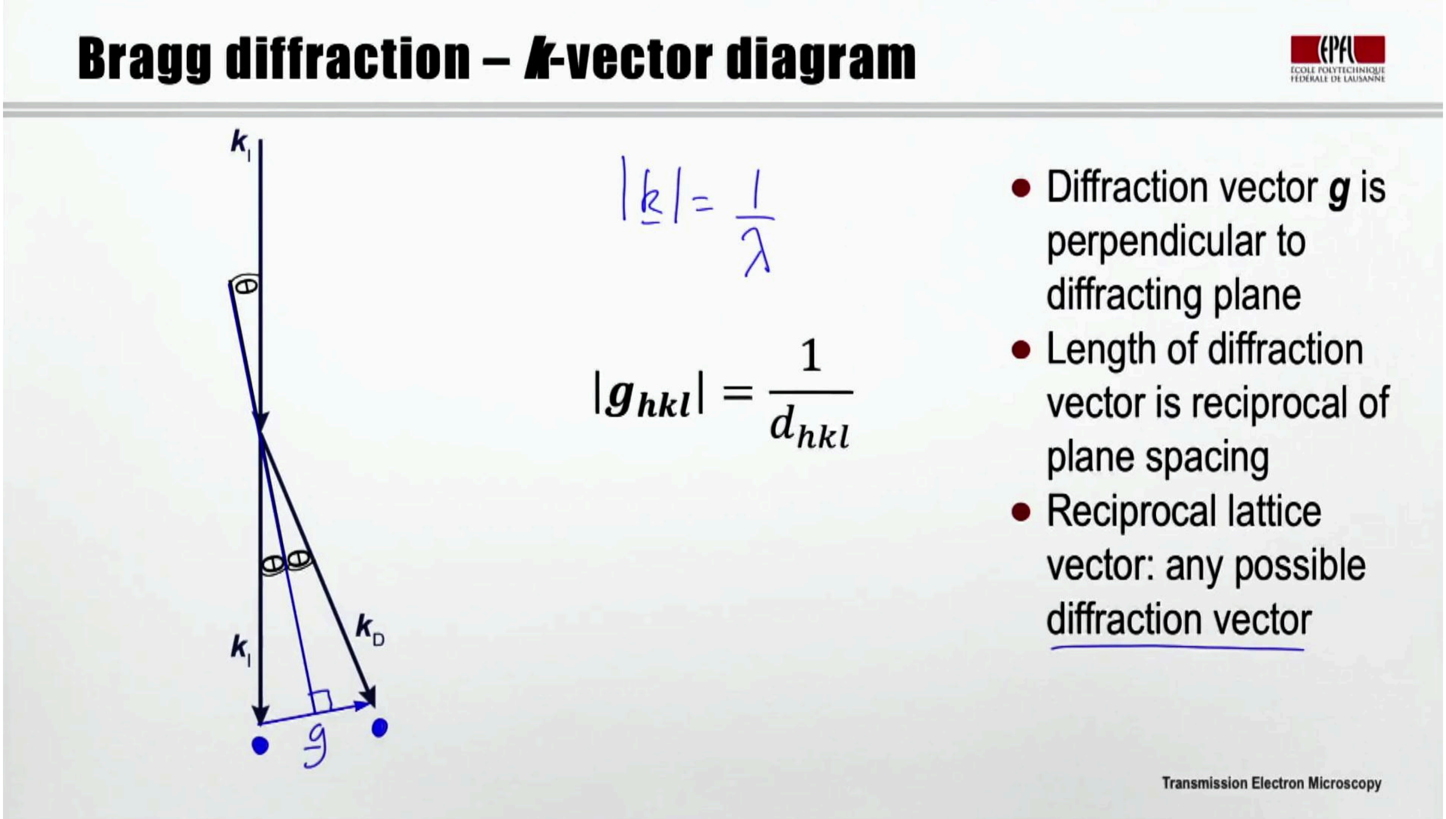


As a way towards understanding the reciprocal lattice, I'm first going to look at the wave vector diagram for two-beam Bragg diffraction, that I discussed in the last lecture. If you remember, in this diagram we have an incident wave vector k_I, where the modulus of a general wave vector k equals 1 over lambda. As we saw last time, this incident wave vector k is scattered at an angle theta, by the Bragg diffracting plane. Such that in the diffraction pattern, we would see two spots: one for the direct beam, corresponding to the incident wave vector k_I, and another spot for the diffracted beam, corresponding to the diffraction wave vector k_D. And then, joining these two, I introduced the diffraction vector g, where I use g as a shorthand for g_hkl. Now if we look at this diffraction vector g, we can notice two things. The first thing, if we just consider that Bragg diffracting plane, it is evident that the direction of the diffraction vector g is perpendicular to the Bragg diffracting plane. Further we saw how the modulus of g is one divided by the plane spacing. While, in this case, g corresponds to a particular diffraction vector, I'm now going to introduce a general vector – called the reciprocal lattice vector – which will correspond to any possible diffraction vector.

Notes

Summary

1m 08s

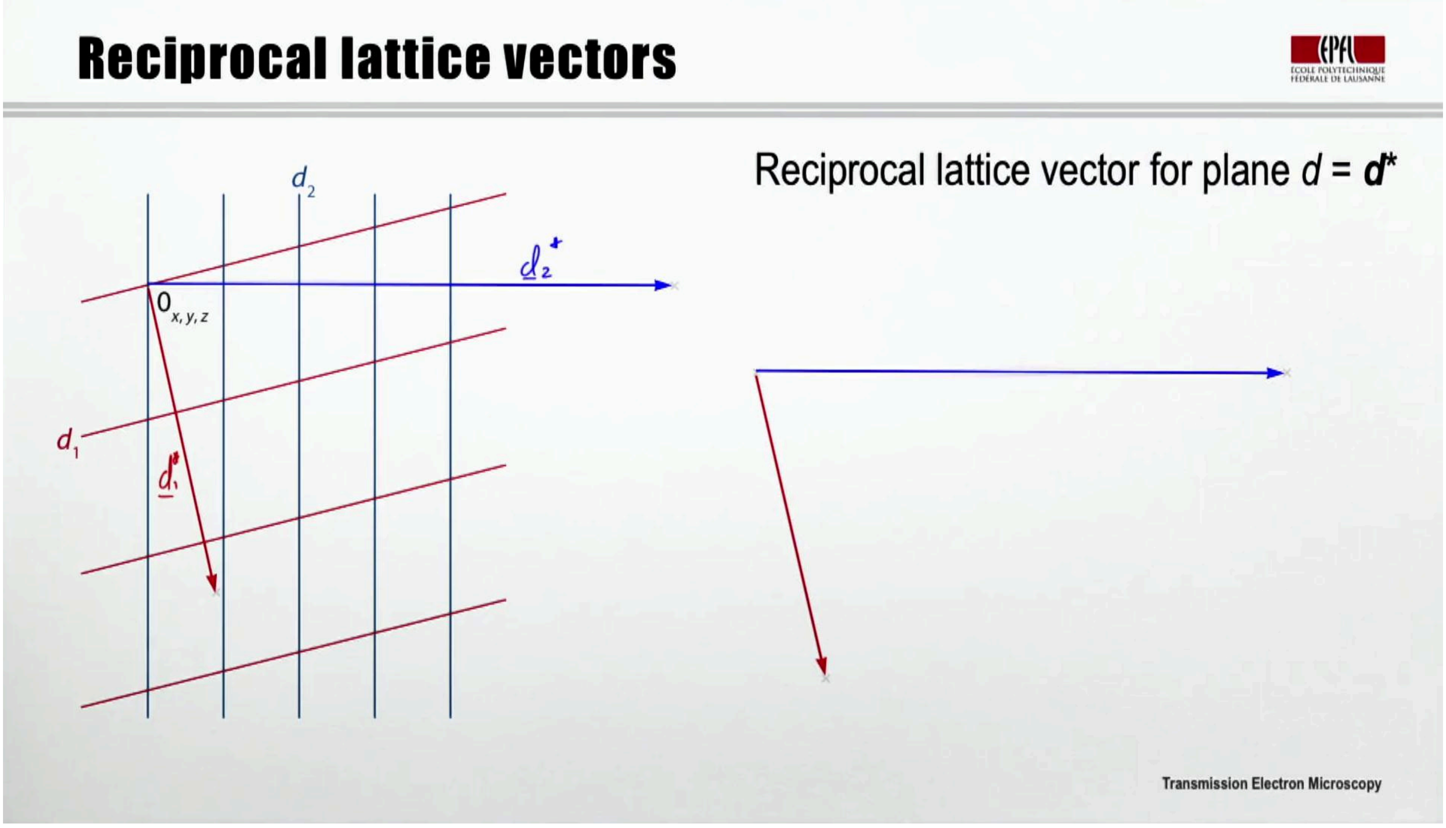


So, each plane (h k l) will have its own reciprocal lattice vector. Evidently, this reciprocal lattice vector must have the same properties as g. In other words, the reciprocal lattice vector will be perpendicular to its plane (h k l), and will have a length which is inversely proportional, or the reciprocal, of the plane spacing.

Notes

Summary

2m 41s

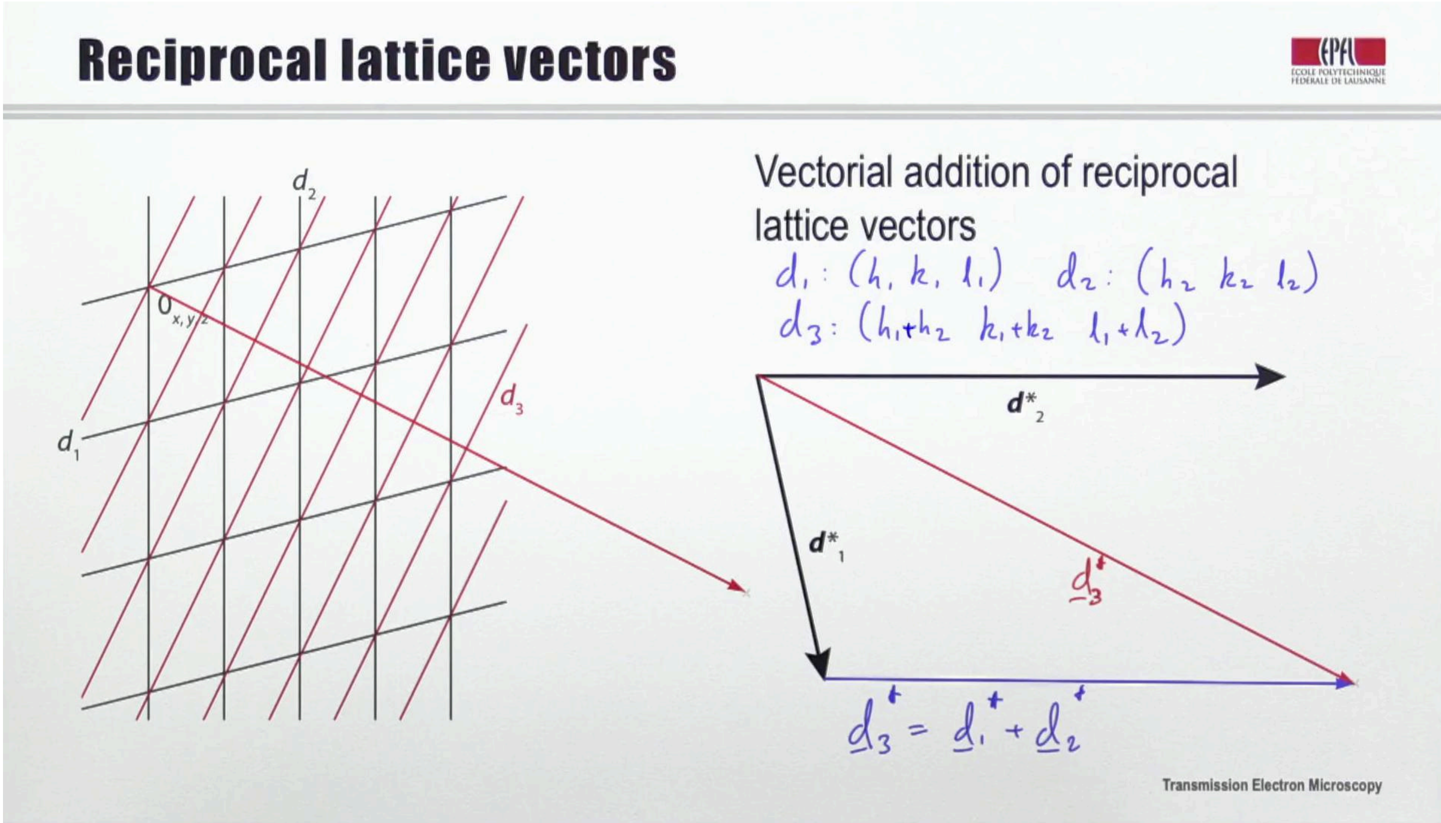


To understand reciprocal lattice vectors, I'm going to draw in some reciprocal lattice vectors for hypothetical planes in real space, such as we have in this diagram here. Where we have plane d_1 in red, and plane d_2 in blue, with an origin here. We are going to define a reciprocal lattice vector for a plane d as d-star. Now, first considering the plane d_1, we know that the reciprocal lattice vector will be perpendicular to the plane d_1, and so, for instance, starting at the origin, will look like this. Now, instead considering the reciprocal lattice vector for the plane d_2, firstly this is going to be perpendicular to that plane d_2, so in a different direction to d_1-star, but also we can see that the plane spacing for d_2 is smaller than the plane spacing for d_1. So for d_2-star we will obtain a longer reciprocal lattice vector, like this. Just for clarity, I will now redraw these two reciprocal lattice vectors over here, so we have d_2-star, perpendicular to the plane d_2, and d_1-star, perpendicular to the plane d_1. These are just the reciprocal lattice vectors for two planes, but we can continue on considering other planes.

Notes

Summary

3m 06s



So we shall do that here. Here I have again marked on the planes d_1 and d_2, and their reciprocal lattice vectors d_1-star and d_2-star, but now I'm going to add another plane, d_3. Now if the plane d_1 has an (h k l) of (h_1 k_1 l_1), and the plane d_2 has an (h k l) of (h_2 k_2 l_2), the fact that the plane d_3 intersects these two planes at one plane spacing from the origin, means that d_3 will have an (h k l) of: (h_1 + h_2 k_1 + k_2 l_1 + l_2). I am now going to mark in the reciprocal lattice vector for this plane d_3. So once again, of course, this reciprocal lattice vector will be perpendicular to the plane d_3, and have a length which is inversely proportional to its plane spacing. Its plane spacing is even smaller than that of d_1 or d_2, so its reciprocal lattice vector is even longer. Now, this vector can be marked in on this cleaner diagram over here, and there, once we have done that, we can notice something: that the reciprocal lattice vector d_3-star equals the reciprocal lattice vector of d_1-star plus the reciprocal lattice vector d_2-star. Therefore, for this relationship of the planes' Miller indices, we have a vectorial addition that: d_3-star = d_1-star + d_2-star.

Notes

Summary

4m 36s

Basis vectors and reciprocal lattice unit cell

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- Real lattice unit cell basis vectors: $\boldsymbol{a}$, $\boldsymbol{b}$, $\boldsymbol{c}$
- Now define reciprocal lattice unit cell with basis vectors: $\boxed{\boldsymbol{a}^*, \boldsymbol{b}^*, \boldsymbol{c}^*}$

Where:

$$\boldsymbol{a}^* = \boldsymbol{d}^*_{100} \qquad \boldsymbol{b}^* = \boldsymbol{d}^*_{010} \qquad \boldsymbol{c}^* = \boldsymbol{d}^*_{001}$$

$$|\boldsymbol{a}^*| = \frac{1}{d_{100}} \qquad |\underline{b}^*| = \frac{1}{d_{010}} \qquad |\underline{c}^*| = \frac{1}{d_{001}}$$

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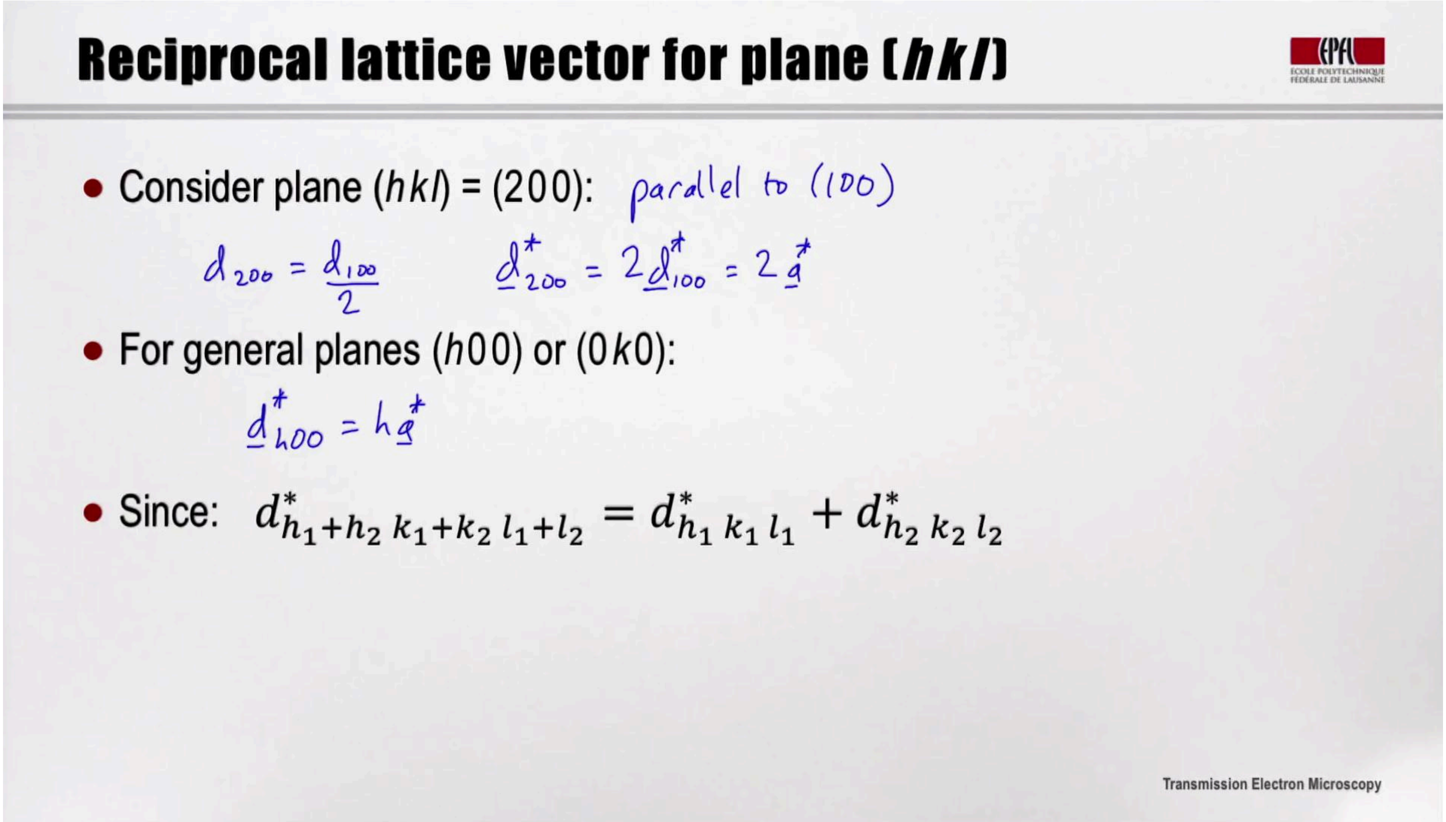
Now we have looked at a general vector for a lattice plane (h k l), we are going to look at the basis vectors that form the reciprocal lattice unit cell. While the real space lattice has unit cell basis vectors a, b, and c in the reciprocal lattice we will also have a unit cell, and this will be defined by its own basis vectors, a-star, b-star, and c-star, defined as follows: that a-star = d-star_100. Clearly, a-star will therefore be perpendicular to the (1 0 0) plane. It will also have a length of one divided by the plane spacing of the (1 0 0) plane. Similarly, b-star = d-star_010, and will have a modulus equal to one divided by the (0 1 0) plane spacing. And we have c-star = d-star_001, where again, the length of c-star equals one divided by the spacing of the (0 0 1) plane.

Notes

Summary

6m 35s



These reciprocal lattice basis vectors can then be used to define the reciprocal lattice vector for a general plane with Miller indices (h k l). To understand why, we can consider the following. First of all, we will consider a plane with Miller indices (h k l) equal to (2 0 0). Now, this (2 0 0) plane is going to be parallel to the (1 0 0) plane. However, if we instead think about plane spacings, we know that the (2 0 0) plane will have a plane spacing which is half that of the (1 0 0) plane. So: d_200 = d_100 divided by 2. Now considering reciprocal lattice vectors, since the planes are parallel, the reciprocal lattice vector for the (2 0 0) plane will be parallel to that of the (1 0 0) plane, but it will have two times the length. So we will have a reciprocal lattice vector: d-star_200 = 2 times d-star_100 Now, as we saw previously, d-star_100 is defined as the reciprocal lattice basis vector a-star. So, d-star_200 simply equals two times a-star. Generalizing this finding a bit further, we go to planes with Miller indices of (h 0 0), or alternatively (0 k 0). Starting with the (h 0 0) plane, taking this derivation a bit further, it can be seen that it has a reciprocal lattice vector: d-star_h00 = h times a-star; the first of the reciprocal lattice basis vectors.

Notes

Summary

7m 44s

Reciprocal lattice vector for plane (hkl)

- Consider plane $(hkl) = (200)$: parallel to (100)

$$d_{200} = \frac{d_{100}}{2} \qquad \underline{d}^*_{200} = 2\underline{d}^*_{100} = 2\underline{a}^*$$

- For general planes $(h00)$ or $(0k0)$: $(00l)$:

$$\underline{d}^*_{h00} = h\underline{a}^* \qquad \underline{d}^*_{0k0} = k\underline{b}^* \qquad \underline{d}^*_{00l} = l\underline{c}^*$$

- Since: $d^*_{h_1+h_2\,k_1+k_2\,l_1+l_2} = d^*_{h_1\,k_1\,l_1} + d^*_{h_2\,k_2\,l_2}$

$$(hkl): \quad \underline{d}^*_{hkl} = \underline{d}^*_{h00} + \underline{d}^*_{0k0} + \underline{d}^*_{00l} = h\underline{a}^* + k\underline{b}^* + l\underline{c}^*$$

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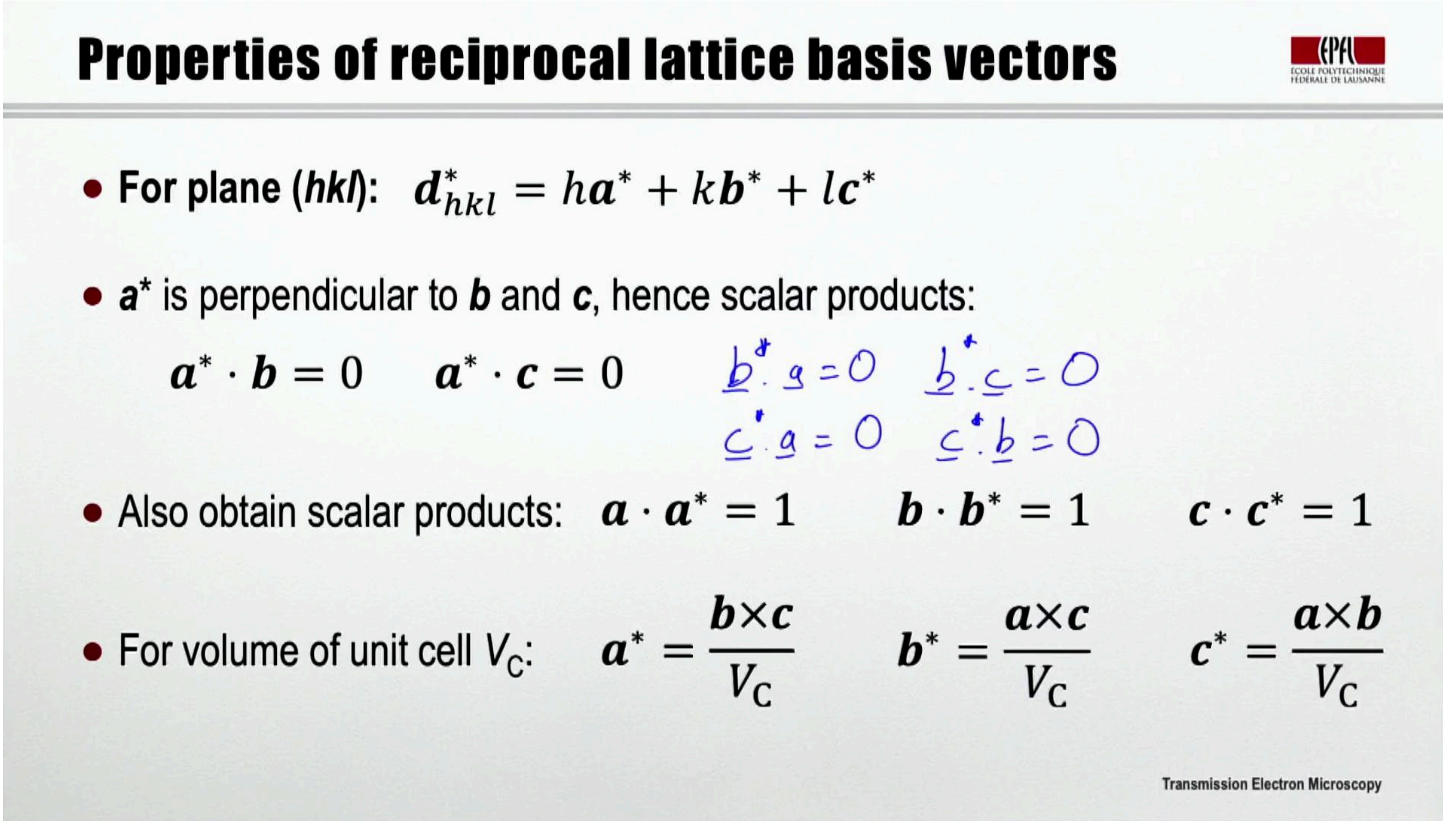
Going on now to the (0 k 0) plane, similarly, that has a reciprocal lattice vector: d-star_0k0 = k times b-star; the second of the reciprocal lattice basis vectors. Finally, we could also consider the (0 0 l) plane. And that in turn, will have a reciprocal lattice vector: d-star_00l = l times c-star. Now taking these findings, together with the vectorial addition for the reciprocal lattice vectors that we saw earlier, for a general plane with Miller indices (h k l) we obtain a reciprocal lattice vector: d-star_hkl = d-star_h00 + d-star_0k0 + d-star_00l, so equal to h times a-star + k times b-star + l times c-star. Thereby relating this plane's reciprocal lattice vector to the Miller indices (h k l) and the reciprocal lattice basis vectors a-star, b-star and c-star.

Notes

Summary

9m 47s

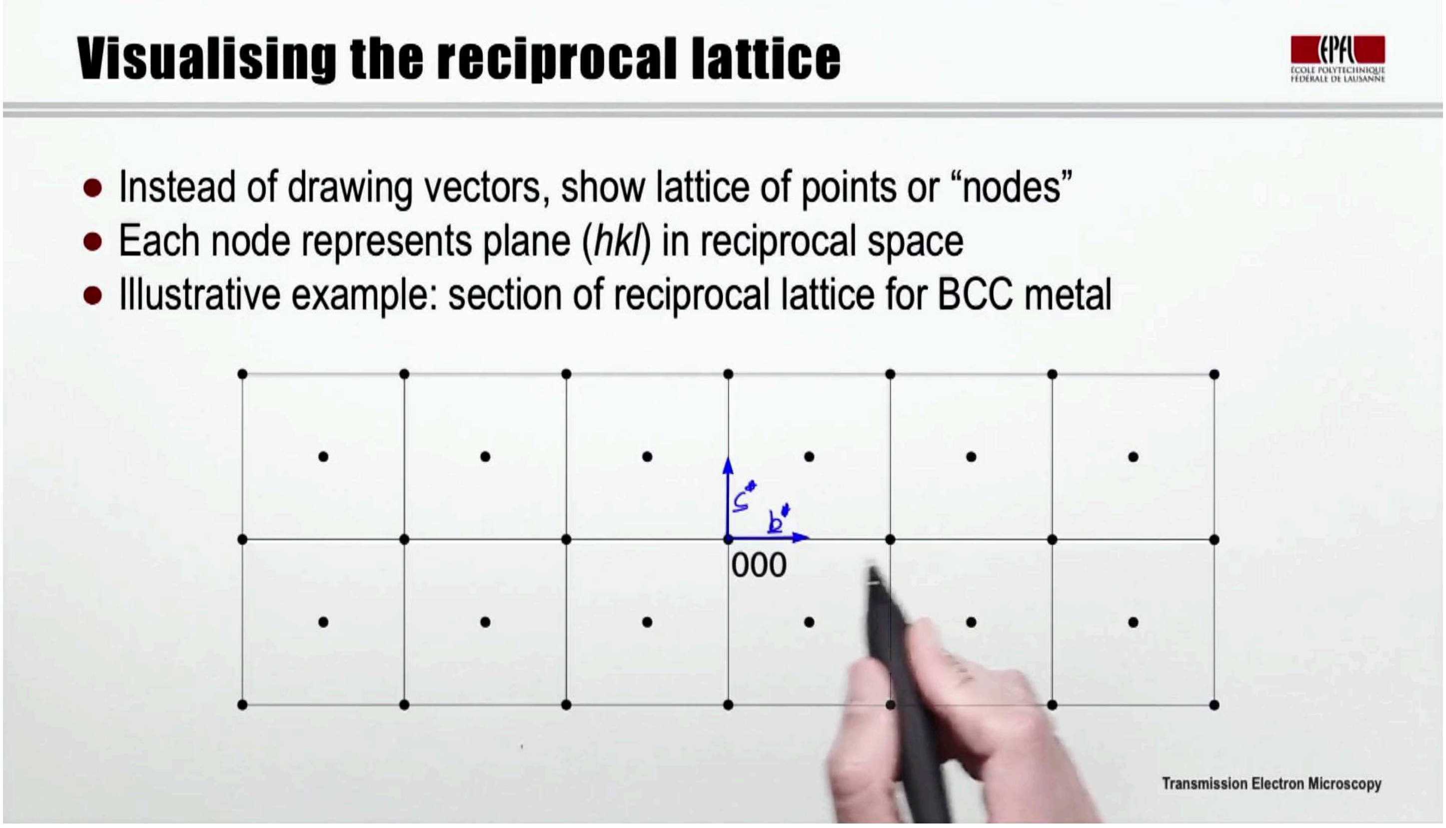


On this slide we will now look in a bit more detail at these properties of the reciprocal lattice basis vectors. Already, we have established that: d-star_hkl = h a-star + k b-star + l c-star. We also know that a-star is the normal to the plane, which contains the real lattice axes b and c. Hence we will obtain the scalar products a-star. b = 0 and a-star. c = 0. Equally: b-star. a = 0, b-star. c = 0, and c-star. a = 0 and c-star. b = 0. It can also be easily obtained that: a. a-star = 1, b. b-star = 1, and c. c-star = 1. Finally, because a-star is perpendicular to b and c, it is clear that a-star is going to be parallel to b cross c. And with a bit more derivation, it can be shown that: a-star = b cross c divided by V_c, where V_c is the volume of the unit cell. And similarly for b-star and c-star.

Notes

Summary

11m 26s

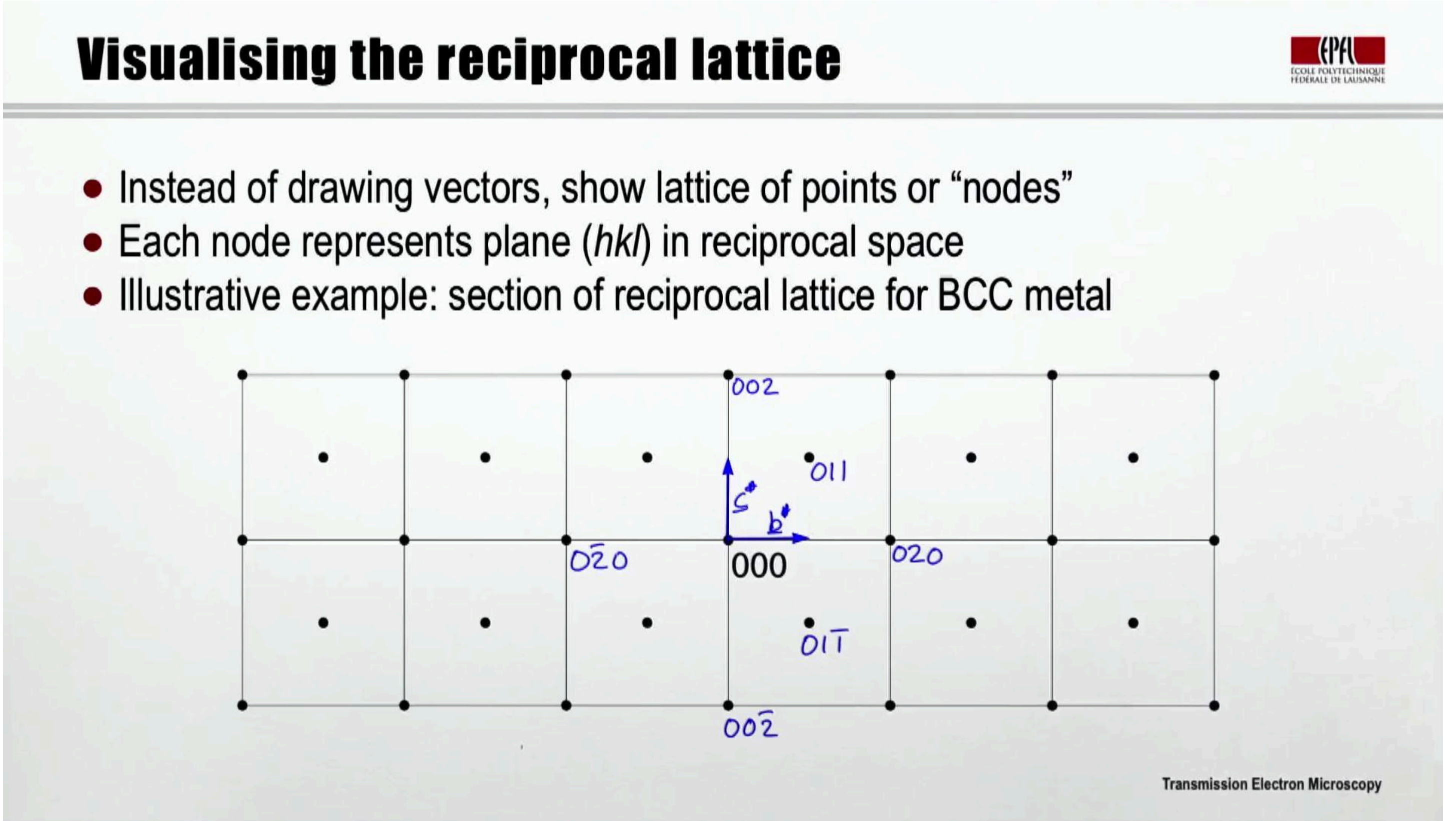


The previous slides have introduced the logic behind the reciprocal lattice vector and discussed the derivation of the reciprocal lattice basis vectors a-star, b-star and c-star. However, what is more important in the lectures to come, is to understand the reciprocal lattice as something visualized by a series of reciprocal lattice nodes, where each node represents the reciprocal lattice vector for a plane (h k l) in what we will call reciprocal space. To illustrate this idea, I'm going to show a section of a reciprocal lattice for a BCC metal. In the middle we have the origin 0 0 0. I'm now going to say that the basis vector b-star lies along here, and has this length. And that the basis vector c-star is here. Because it is cubic, the lengths of b-star and c-star are identical to each other, and they have a 90-degree angle between them. Now considering the systematic absences for BCC, if we go along the vector b-star, then the first diffracting plane we can have with a normal parallel to this vector will be the (0 2 0) plane. And we know that the (0 2 0) plane will have a diffraction vector which will be two times the length of b-star, since b-star corresponds to d-star_010.

Notes

Summary

12m 41s

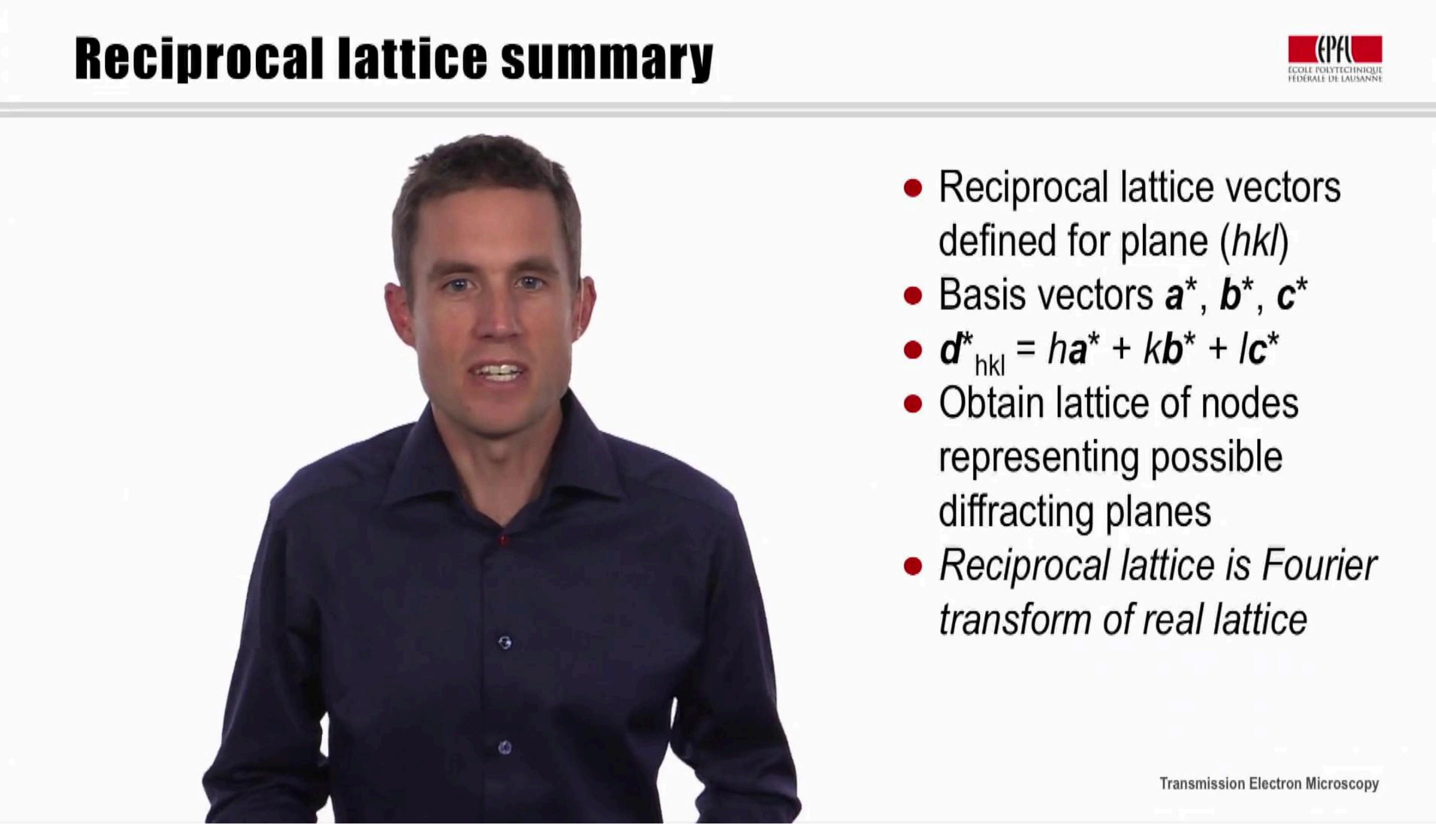


Therefore, we represent the reciprocal lattice vector for that (0 2 0) plane as a node here. Note that rather than drawing a vector to that node, we just represent it as a spot, which corresponds to a possible diffraction event. If that is the node for the (0 2 0) plane on this axis – parallel to c-star – we will have the 0 0 2 node here. Between them, we will have another node, for the (0 1 1) plane. We can carry on identifying these different nodes. By symmetry, here we will have the 0 0 –2 and here the 0 –2 0. Here, the 0 1 –1, and so on. Now for simplicity, this is just a two dimensional section of what would be a three dimensional lattice. And we will see next time how, by interacting this three dimensional lattice with the Ewald sphere, we can identify which planes are going to diffract under certain conditions of, for instance, sample orientation with respect to the electron beam.

Notes

Summary

14m 04s



To summarize, I have introduced the concept of the reciprocal lattice vector for a plane (h k l). And further seen how this reciprocal lattice vector d-star_hkl can be described in terms of the reciprocal lattice unit cell basis vectors a-star, b-star and c-star. Further to that, by assigning the reciprocal lattice vector for each plane a node, we can consider schematically a three dimensional reciprocal lattice made up of a framework of nodes, where each of these nodes represents a possible diffracting plane. Finally, as a last note, I will point out that the reciprocal lattice is in fact the Fourier transform of the real lattice. And this is something that will become important for understanding the nature of electron diffraction in a few lectures time.

Notes

Summary

15m 16s