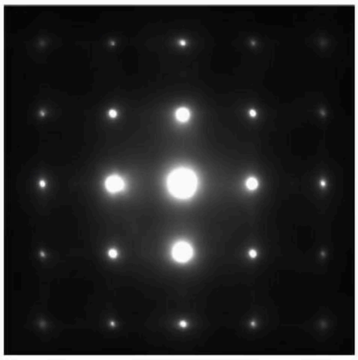
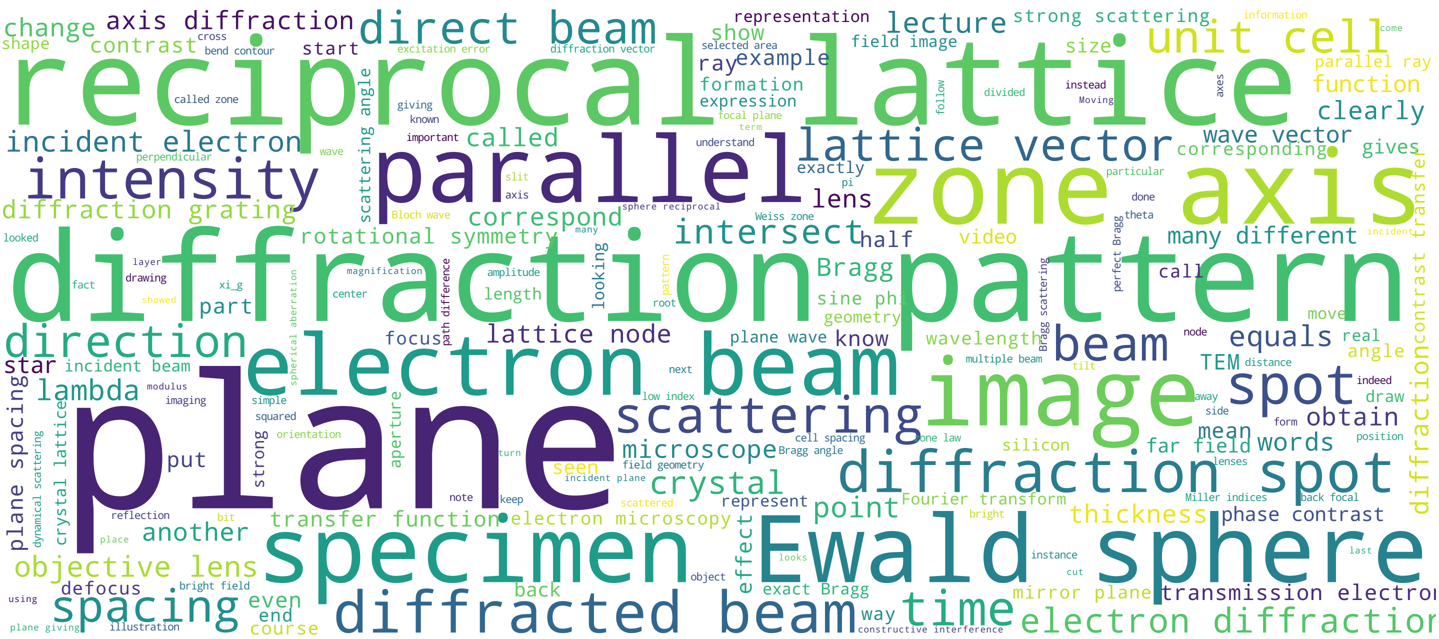


Basics of ED: multiple beam scattering

Transmission Electron Microscopy

Prof. C. Hébert & Dr D. Alexander



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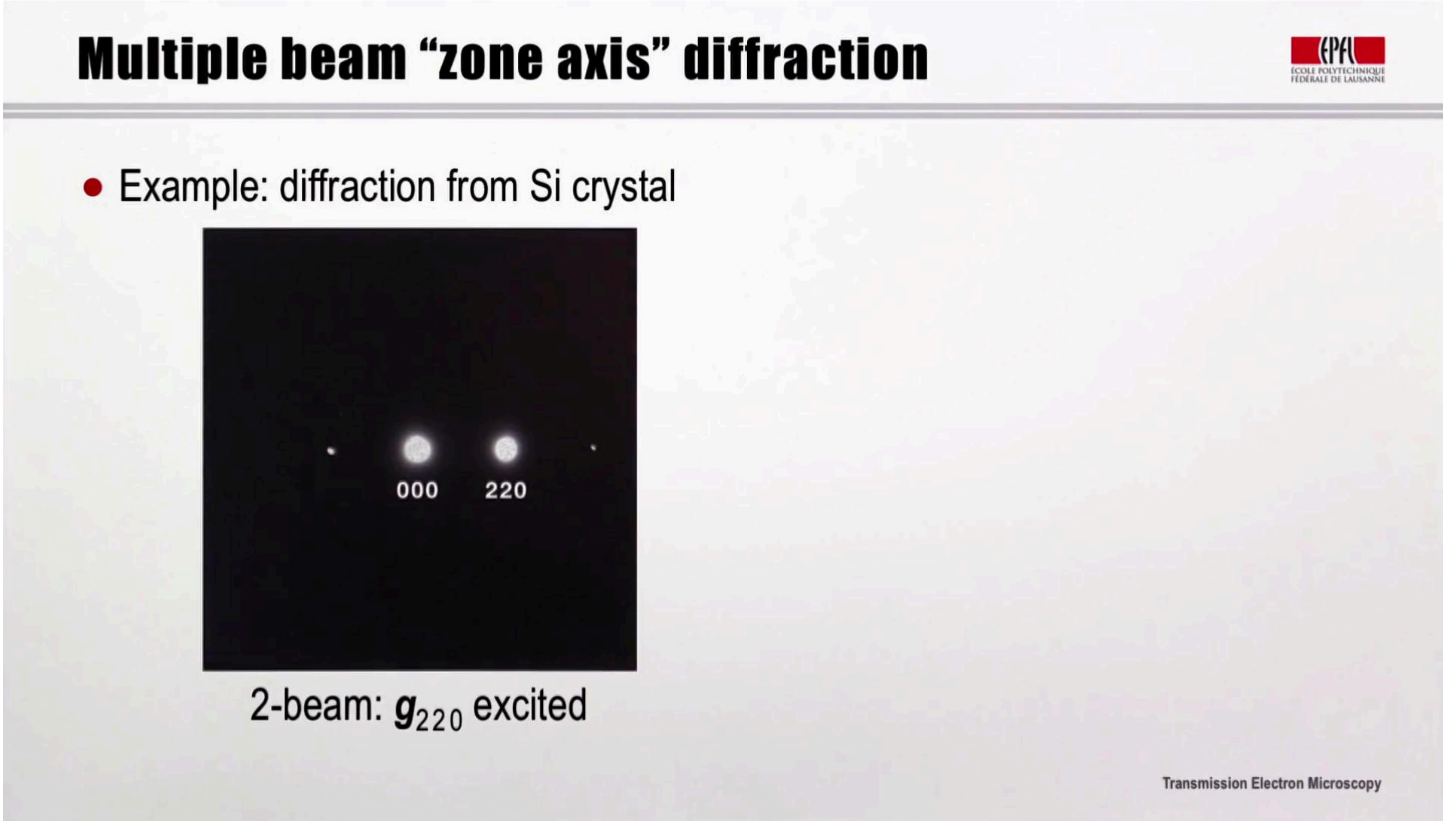
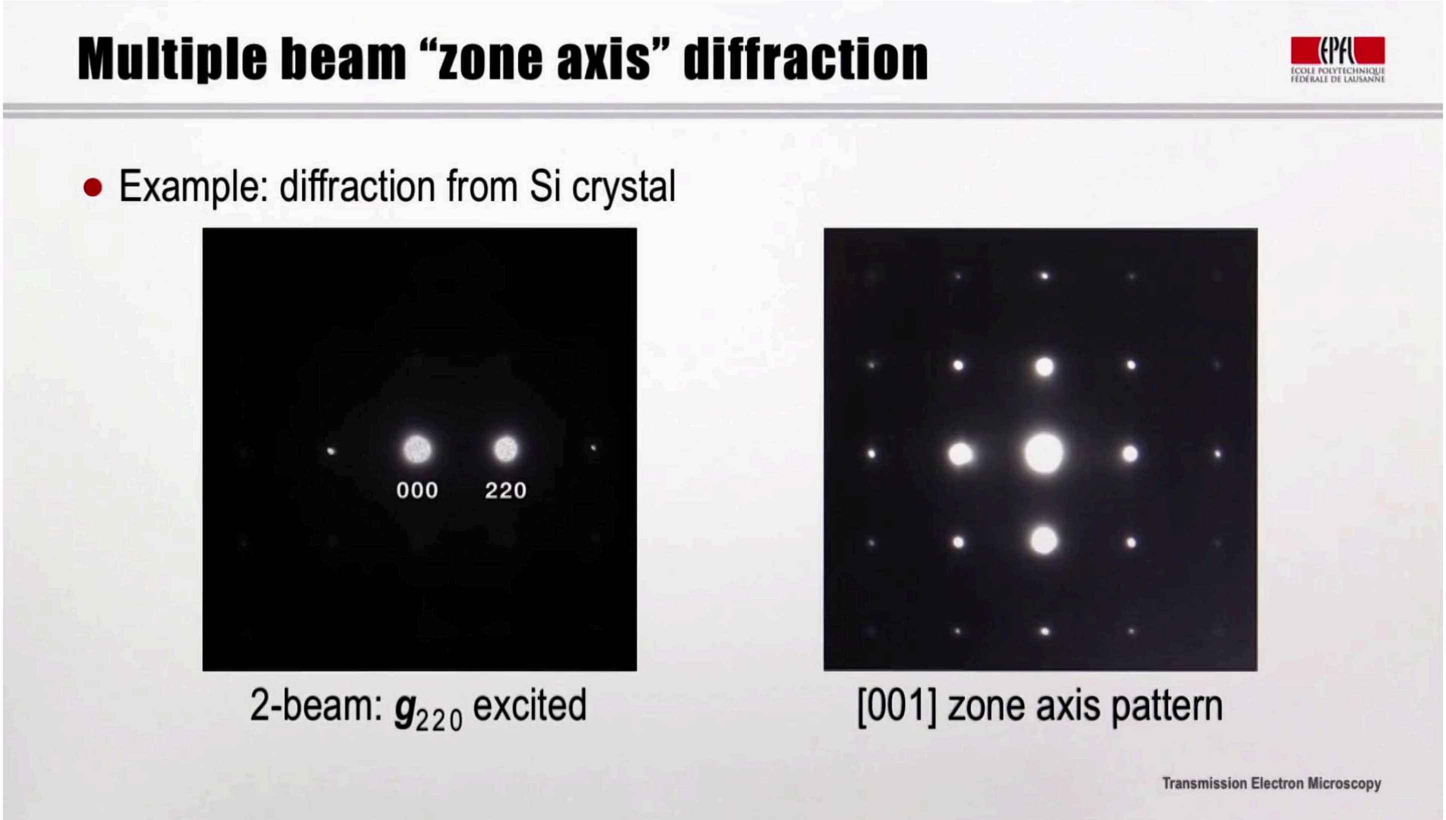


Welcome to CIME's lectures on transmission electron microscopy for materials science. In the last few lectures on the basics of electron diffraction, I have looked at the theoretical case of two-beam electron diffraction. As we saw, in this case, we have one plane (h k l) which is inclined relative to the incident electron beam, at the exact Bragg angle, theta_B. We have strong scattering from that plane, giving a diffraction pattern which has two strong spots: one for the direct beam, the 0 0 0, and another for the diffracted beam, h k l. However, if we look back at the video of electron diffraction I showed in my first lecture, you will see in that video that there is another case of diffraction where we have many different diffraction spots – so scattering from many different beams – also showing a high degree of symmetry. This is a so-called zone axis diffraction pattern, and this is the case that I'm going to look at in this lecture. As an example, we can look at two experimental diffraction patterns taken from a single crystal of silicon. In this pattern, I once again show the case of two-beam electron diffraction, here with the plane with Miller indices (h k l) of (2 2 0) at the exact Bragg condition. So, we have strong scattering into this diffraction spot, such that we have strongly excited the diffraction vector g_220.

Notes

Summary

0m 05s

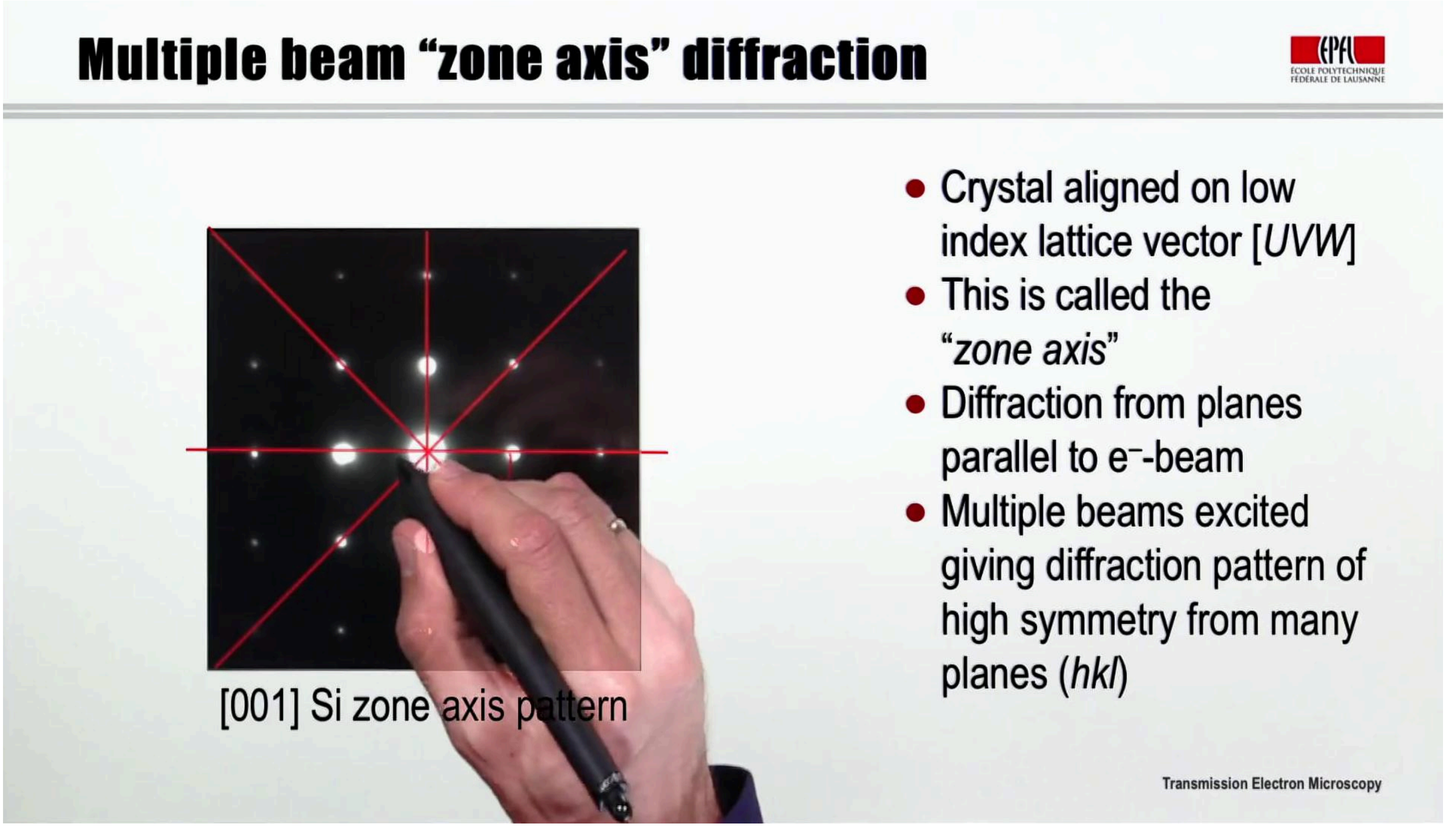


In this case, I have instead aligned the crystal such that its [0 0 1] axis – that is its z axis – is aligned exactly parallel to the incident electron beam. This gives a so-called [0 0 1] zone axis diffraction pattern. We will now look at this case a bit more closely.

Notes

Summary

1m 52s

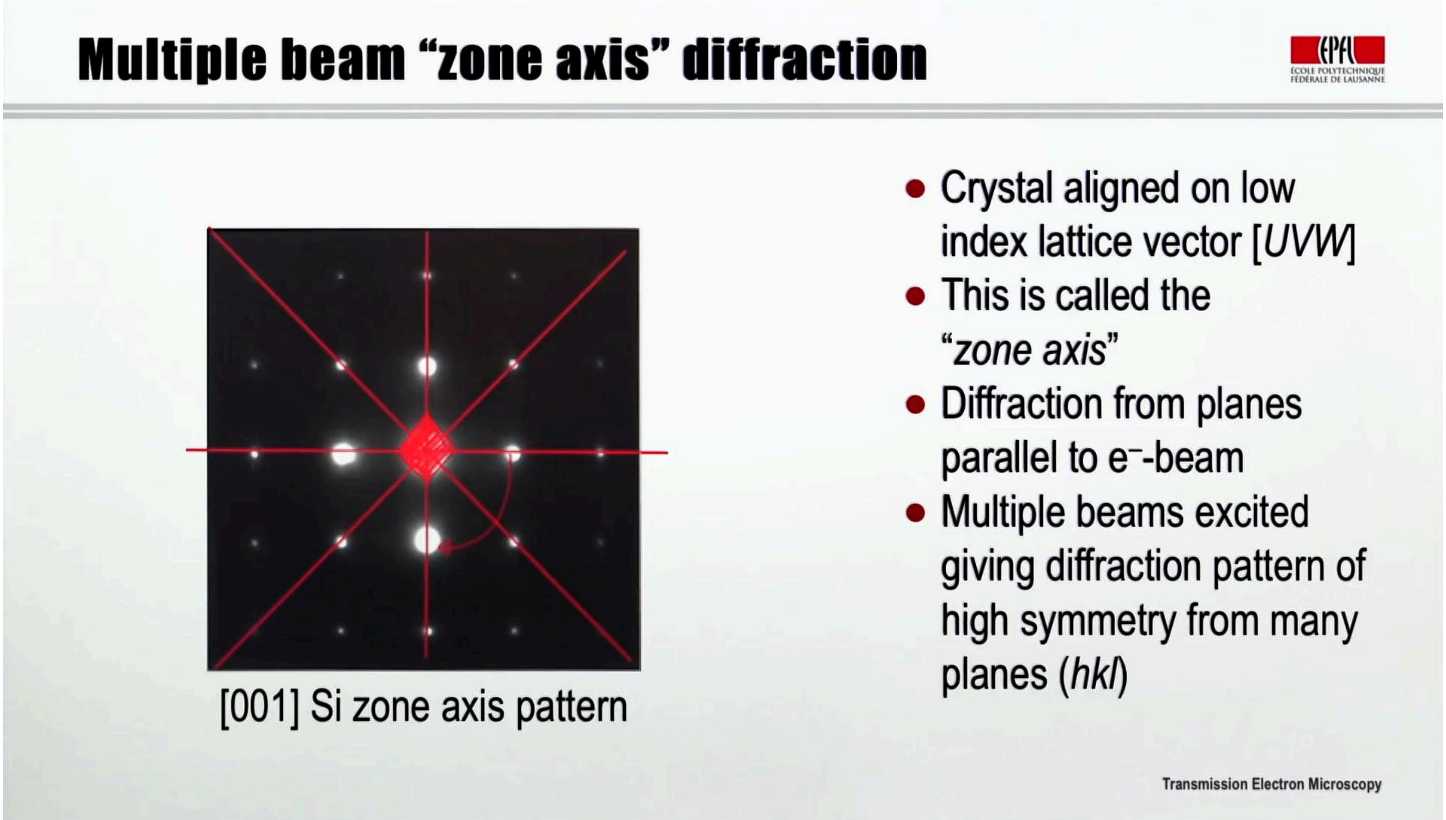


So if we look at this pattern, we can see that we have many different diffracted beams, so-called multiple beam scattering. The crystal has been aligned on what we call a low index lattice vector; effectively an important crystallographic direction. For instance, if you have a cubic crystal, such as silicon, this could be a direction such as: [0 0 1], [1 1 0], or [1 1 1]. This lattice vector will have these indices [U V W], and we will call this the zone axis. So the zone axis corresponds to the direction in the crystal which is aligned parallel to the incident electron beam. In this case, we have diffraction from planes in the crystal which are parallel to that incident electron beam. So to the electron beam these planes look like they are end on, with each plane giving a corresponding diffraction spot. Multiple beams are excited at the same time. In this condition we obtain a diffraction pattern which has lots of symmetry. So if we look at this pattern in particular, we can see that we have a mirror plane here, a mirror plane here, another mirror plane here, and a fourth mirror plane here. Instead looking at rotational symmetry we can see that there is 90 degree rotational symmetry for all the diffracted beams.

Notes

Summary

2m 16s

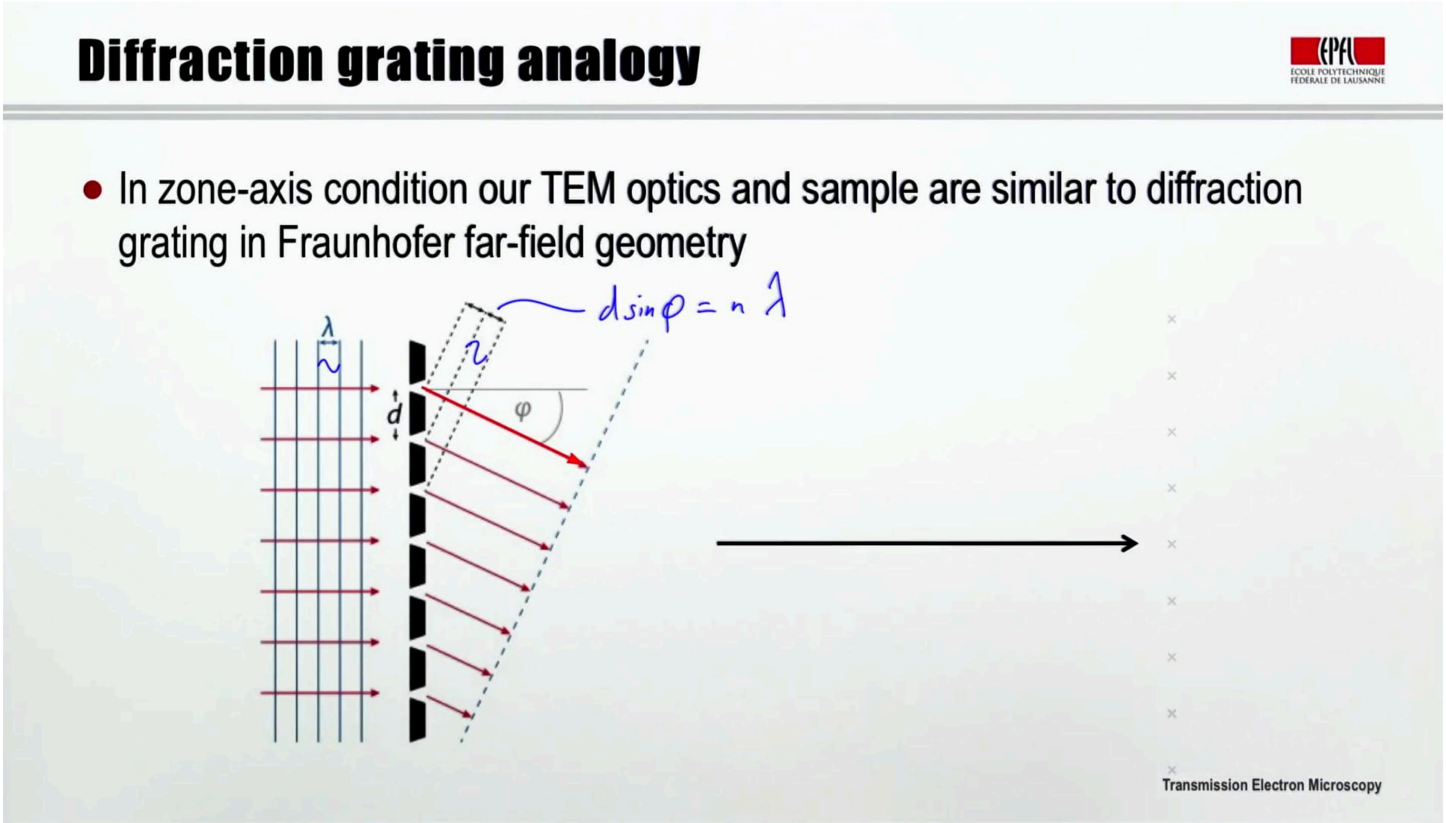


So, we have fourfold rotational symmetry: a tetrad. And we can observe that this mirror and rotational symmetry corresponds to the rotational symmetry for the [0 0 1] direction in the crystal. In other words, we have a diffraction pattern which has the rotational and mirror symmetry of its corresponding lattice vector in the real space crystal lattice. So why does such a diffraction pattern form in this zone axis condition?

Notes

Summary

3m 42s

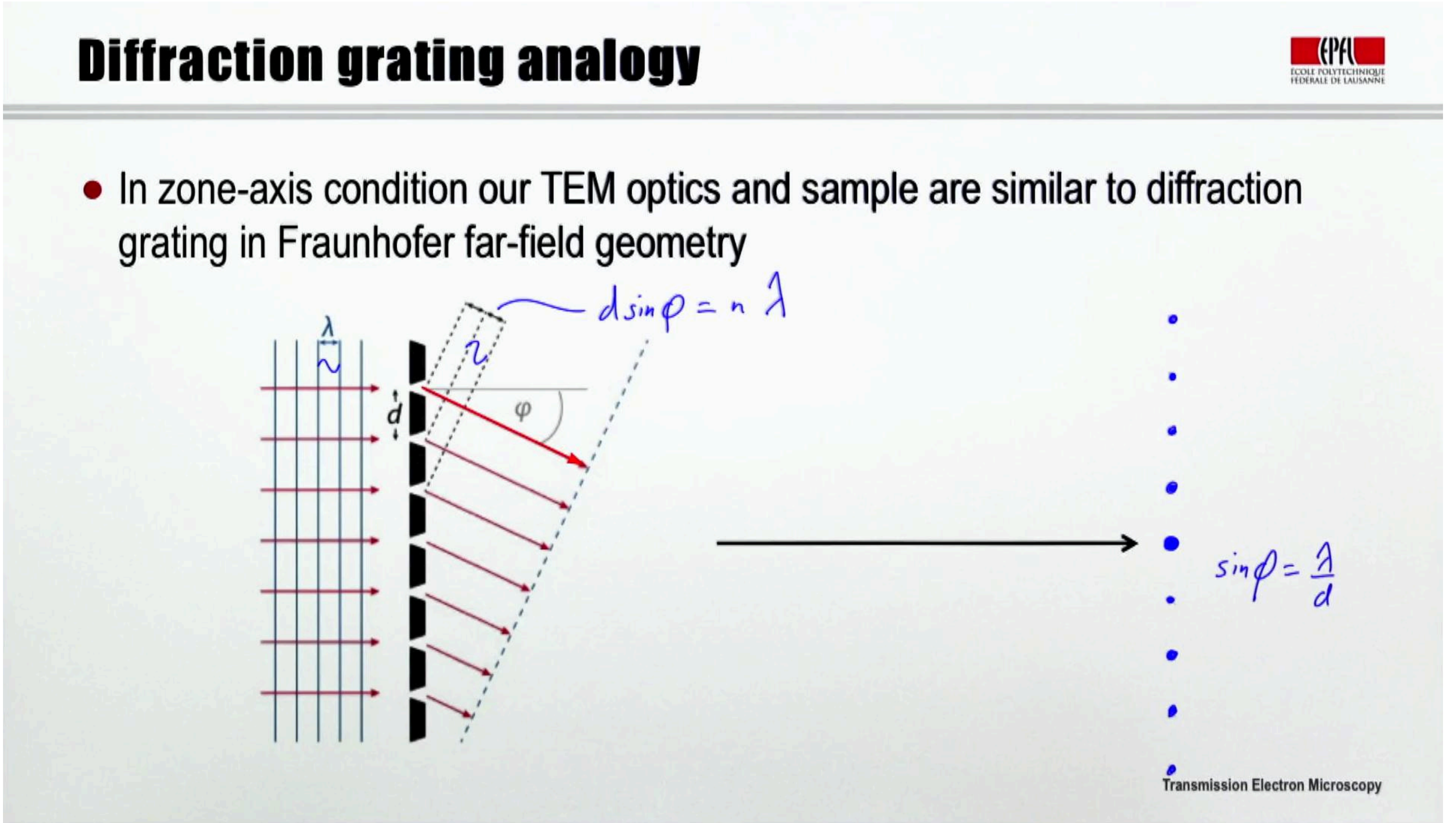


To gain some insight into the formation of this zone axis diffraction pattern, I'm going to make a simple analogy, and say that in this zone axis condition our TEM optics and sample are similar to the condition for a diffraction grating in Fraunhofer far-field geometry. Here I have a representation – an illustration – of this diffraction grating, and we can see that we have an incident plane wave, with a wavelength lambda, being scattered by a regular array of slits, with each slit having the spacing d. When this incident plane wave is scattered by the grating, each slit acts as the source of a spherical wavelet spreading out. We can represent that wavelet as a ray scattered at different angles, which here are called phi. Now what we can see is that, at certain angles phi, parallel rays have a path difference which will correspond to that for constructive interference. In other words, this path difference here – which equals d sine phi – corresponds to one, or multiples of, a wavelength. In other words we have constructive interference when: d sine phi = n times lambda, where lambda is the wavelength and n is an integer.

Notes

Summary

4m 12s

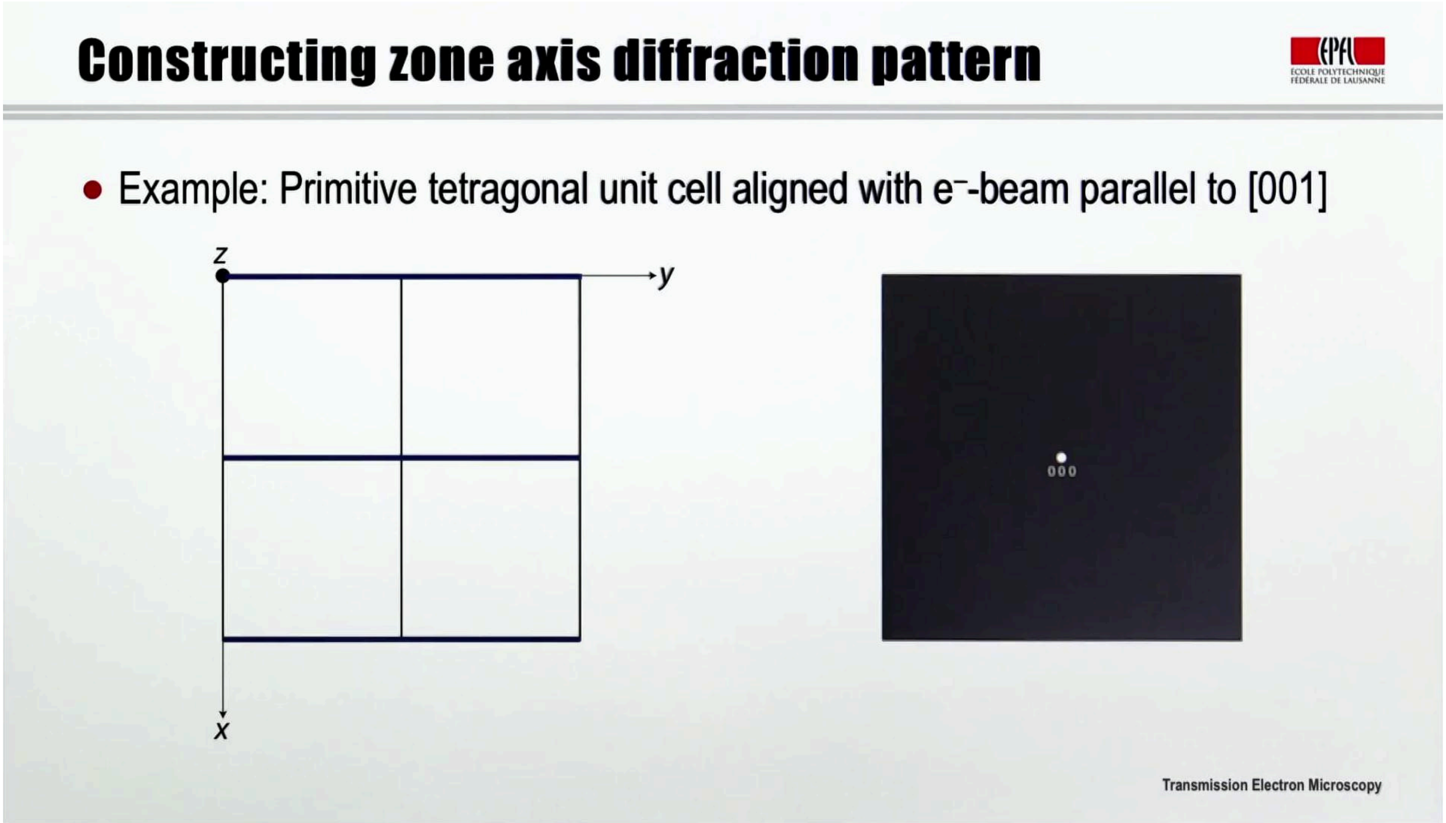


If we now put a screen sufficiently far from this diffraction grating, then we will be in a far-field geometry, where parallel rays come to a point. And we will obtain a diffraction pattern, where first of all we will have a spot in the center corresponding to beams that are scattered straight on: the direct beam. But then, for sine phi = lambda over d, we will obtain another diffraction spot, here. So with an angle of scattering given by sine phi = lambda over d. Then we will have another spot here, for 2 lambda over d, 3 lambda over d, and so on, and their inverses the other side. So you can see that this grating has given a diffraction pattern of regularly spaced spots. As an exercise, you can prove to yourself that, in the small angle approximation for this far-field geometry, the angle of scattering between the diffraction spots is exactly the same as you would obtain for Bragg diffraction in an electron diffraction pattern. We should also note that this Fraunhofer far-field case is equivalent to the back focal plane of the objective lens in TEM because, in both cases, parallel rays come to a point. We shall now use this diffraction grating approximation to help construct a zone axis diffraction pattern.

Notes

Summary

5m 41s

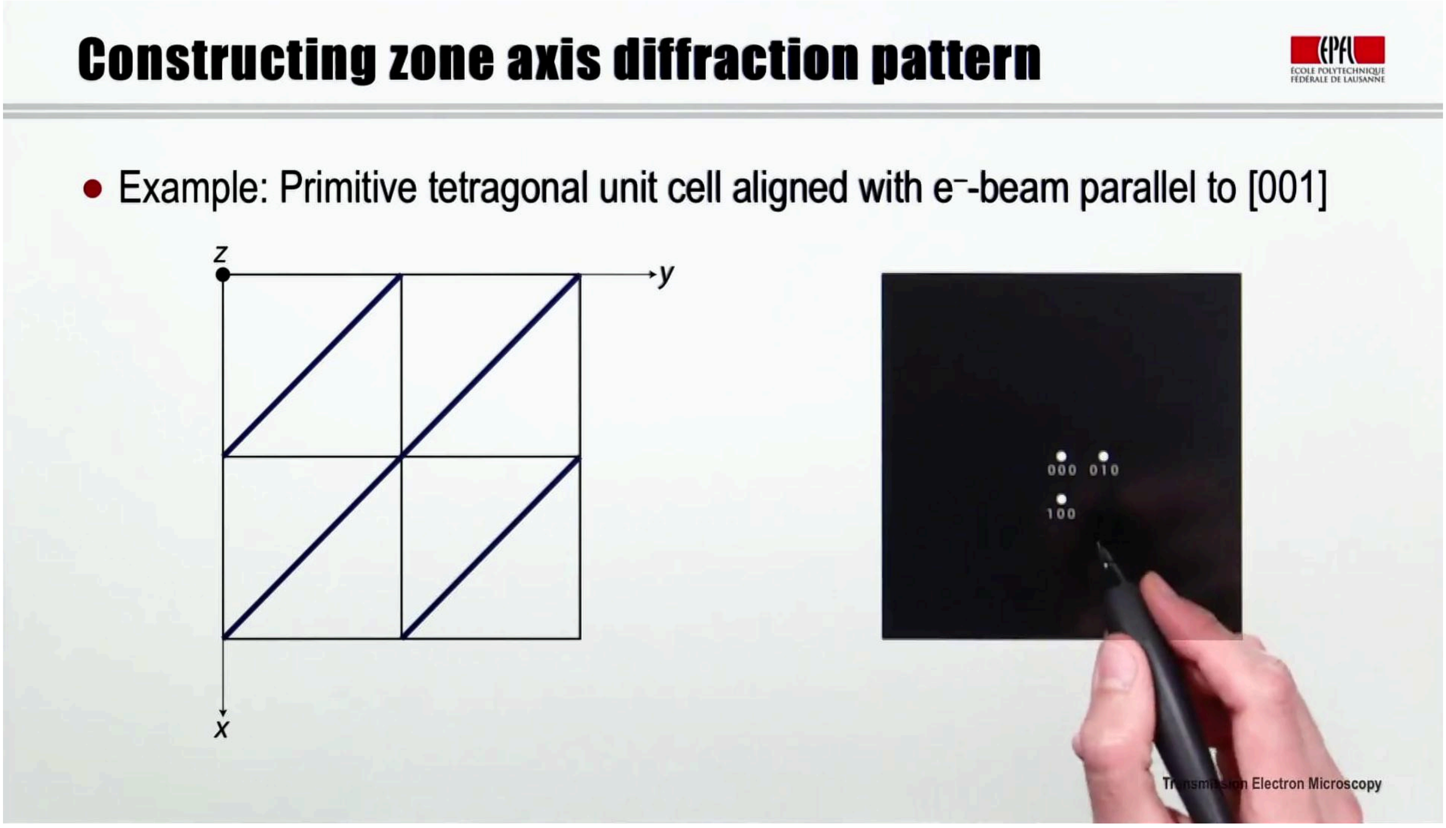


For this example, I'm going to take a very simple case of a primitive tetragonal unit cell, such that there are no systematic absences in the reciprocal lattice. And, we are going to take an alignment of this tetragonal unit cell of the electron beam parallel to the lattice vector [0 0 1]. In other words, parallel to the z axis of the unit cell. So here I show an illustration of a two by two block of unit cells in this orientation. Being tetragonal, we have a = b. So, we just have a simple square form. And now we are going to look at the planes which are parallel to the incident electron beam – in other words words the electron beam will view them as end on planes – and take each plane in turn, and say "that is like a diffraction grating" and we will see which diffraction spot it will make in our diffraction pattern. So if we start off even without any object, of course, we will always have a central direct beam in the diffraction pattern, the so-called 0 0 0. Now we consider diffraction from planes. First of all I take this plane here. We can see that this plane is parallel to the y-axis and intersects the x-axis at one unit cell parameter. So this is clearly the (1 0 0) plane.

Notes

Summary

7m 10s

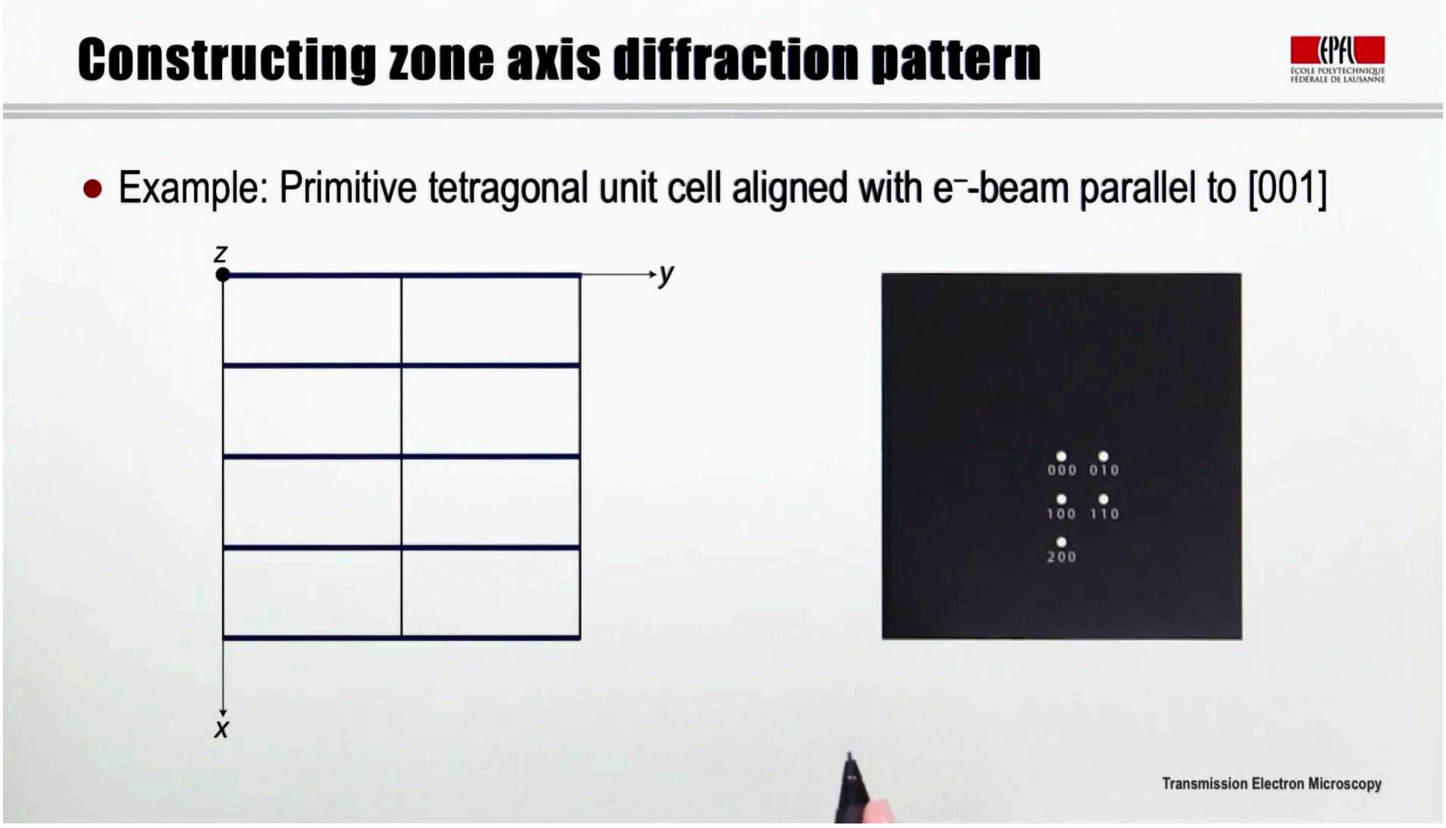


Like a diffraction grating, it will make a diffraction spot in our diffraction pattern perpendicular to that plane and with a spacing which will be the reciprocal of the plane spacing d. So we get a diffraction spot looking like this. Now we move on and consider another plane. We can see that this plane is instead parallel to the x-axis, and intersects the y-axis at one unit cell spacing. So this is clearly the (0 1 0) plane. This plane has exactly the same spacing as the (1 0 0), but it is perpendicular to it. So it will give a diffraction spot over here, with the same spacing as the (1 0 0) but at an angle of 90 degrees. Now we move on, and consider this plane. We can see that this plane intersects the x- and y-axes at one unit cell spacing. So this is going to be (1 1 0) plane. Its spacing is one over root two of the spacing of the (1 0 0) plane, or the (0 1 0) plane. So it is going to give a reciprocal lattice spacing which is root two times larger than this spacing here. Also it is at this angle, here. It is going to give a spot, then, in this direction.

Notes

Summary

8m 37s

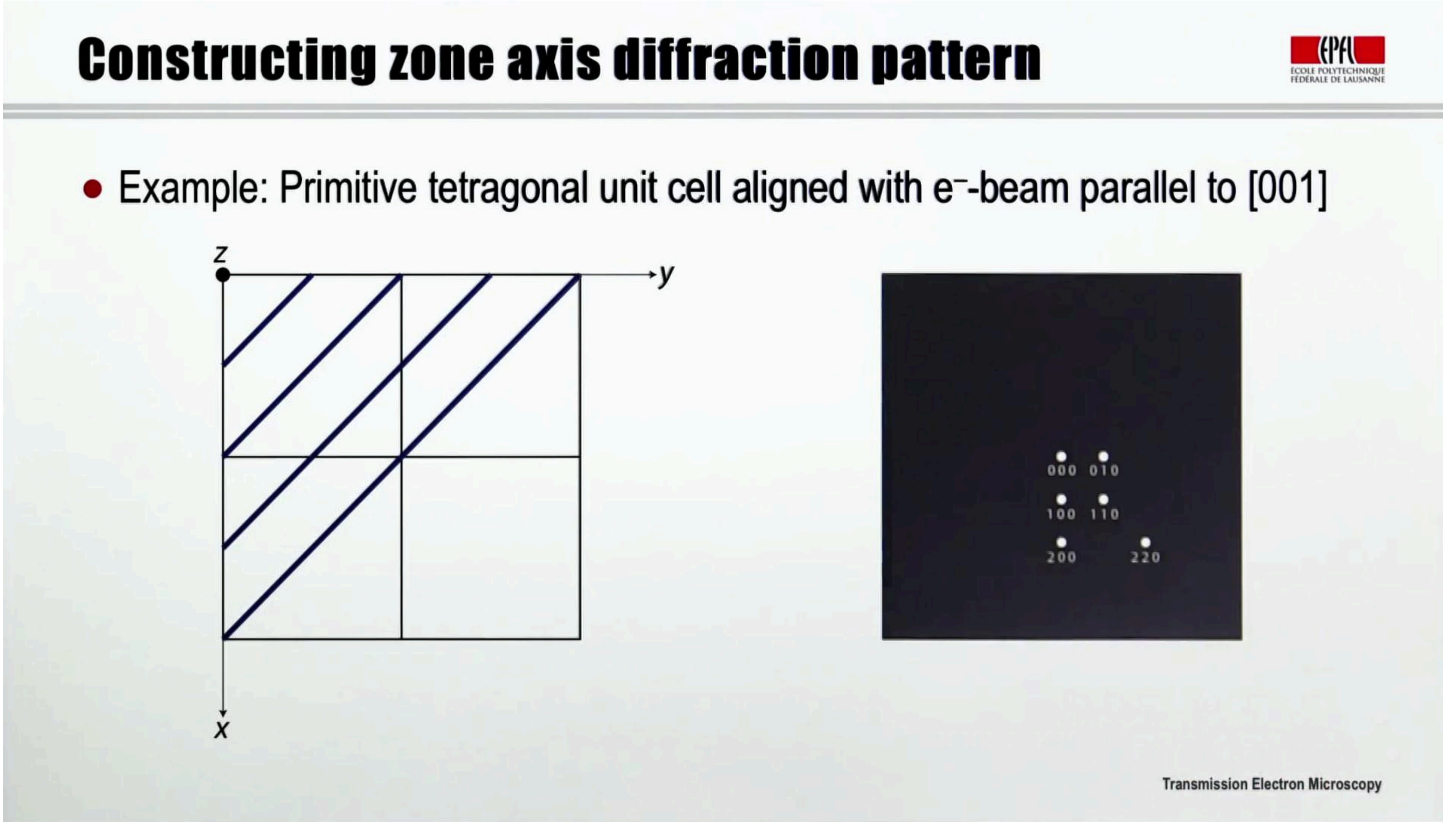


So it is going to give a spot over here: the spot for the (1 1 0) plane. Moving on, I consider this plane. We can see that this plane is parallel to the (1 0 0), but it intersects the x-axis at half a unit cell spacing. So it is going to be the (2 0 0) plane. Being parallel to the (1 0 0), it is going to give a spot in this direction. But, having half the plane spacing of the (1 0 0), the scattering angle will be two times that of the (1 0 0), so it gives a spot here – the (2 0 0).

Notes

Summary

9m 58s

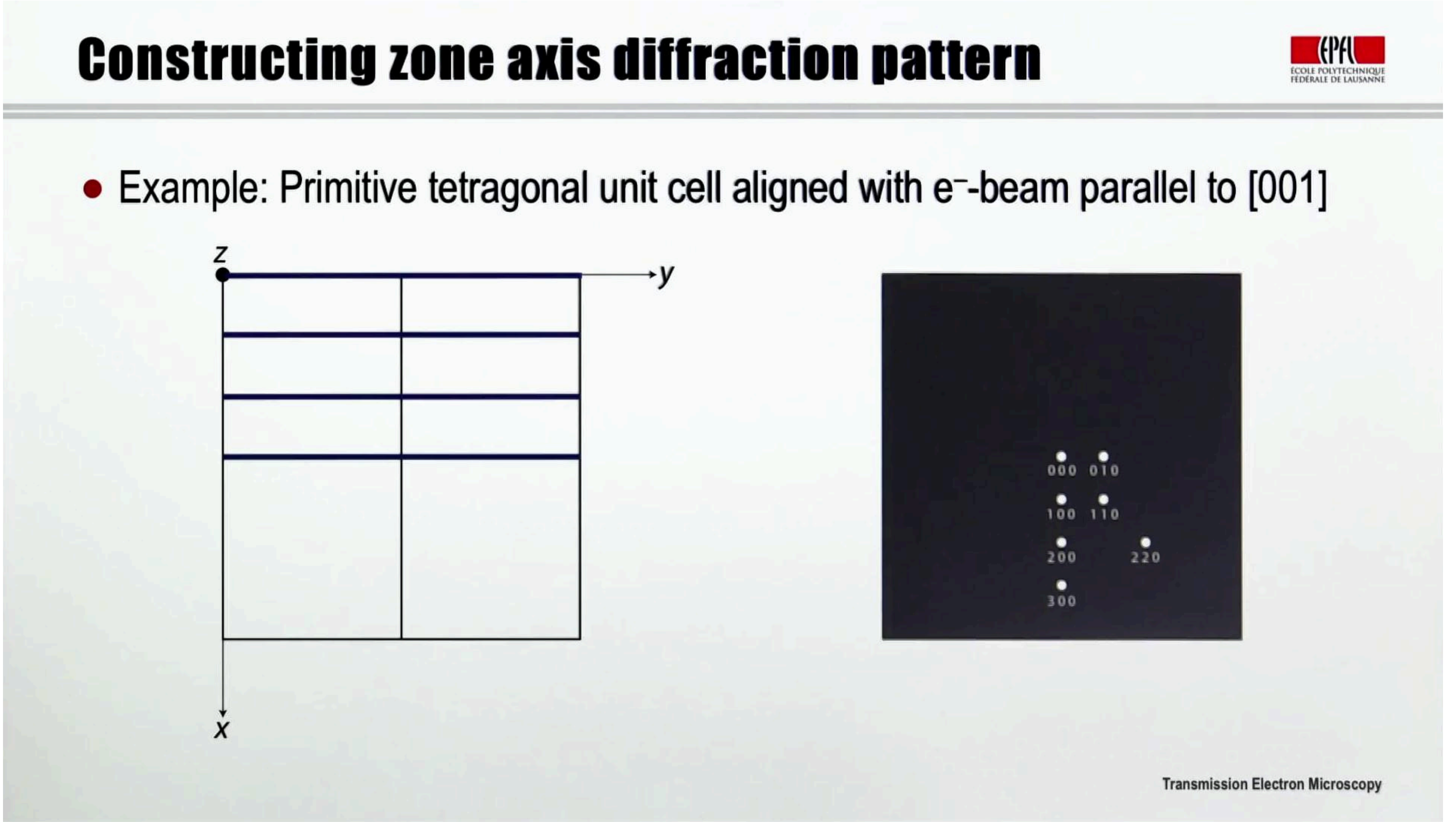


Moving on, I put on this plane here. It intersects at half a on the x- and y- axes, so it is clearly the (2 2 0) plane. Being the (2 2 0), it is going to give a spot parallel to the (1 1 0). But having half the plane spacing, is going to have double the scattering angle, so it will give a spot over here.

Notes

Summary

10m 31s

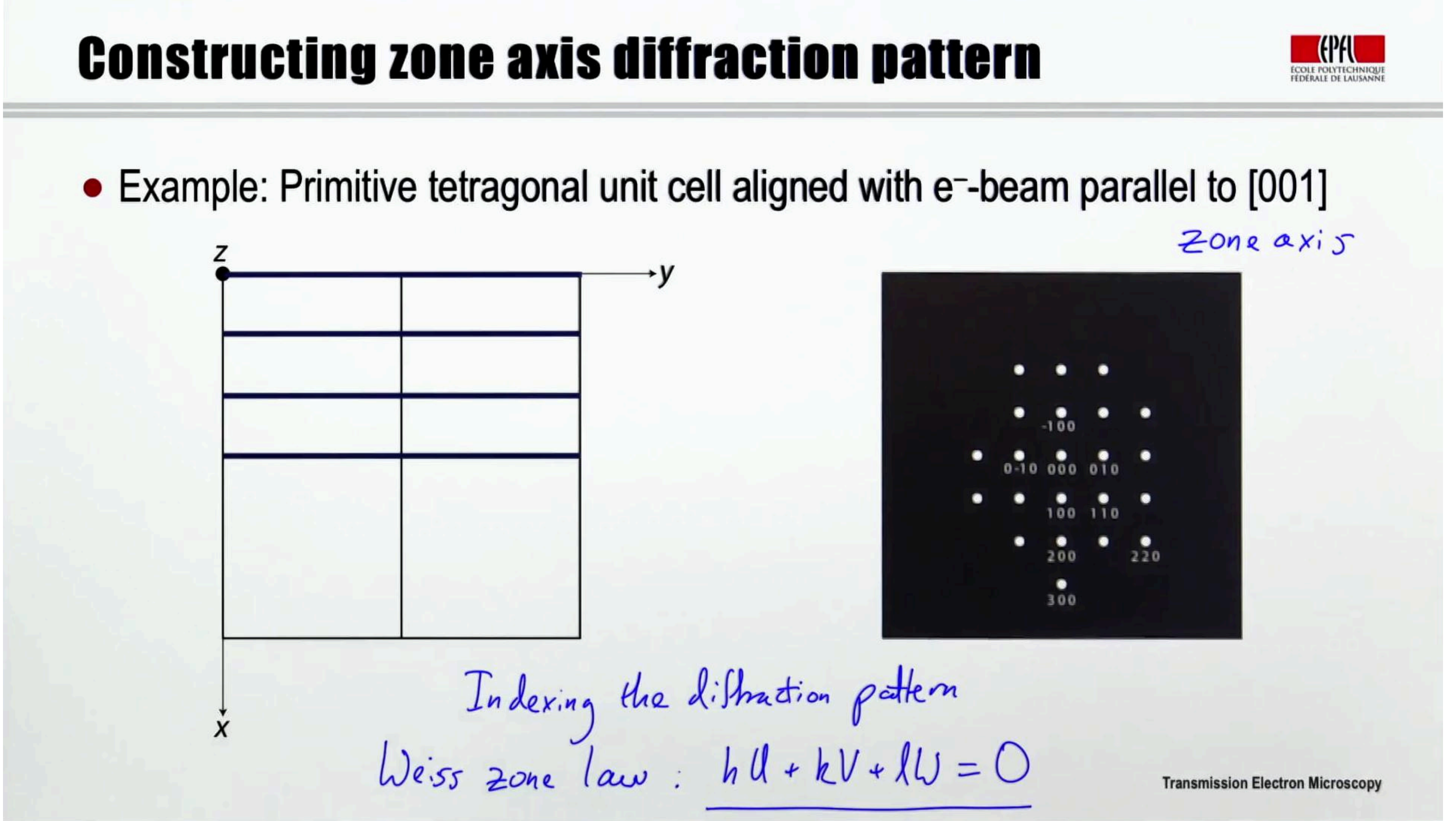


And we can keep on going. Here I've put on the (3 0 0) plane, which of course is parallel to the (1 0 0), so will give a spot in the same direction, but with three times the scattering angle, so giving a spot here.

Notes

Summary

10m 55s

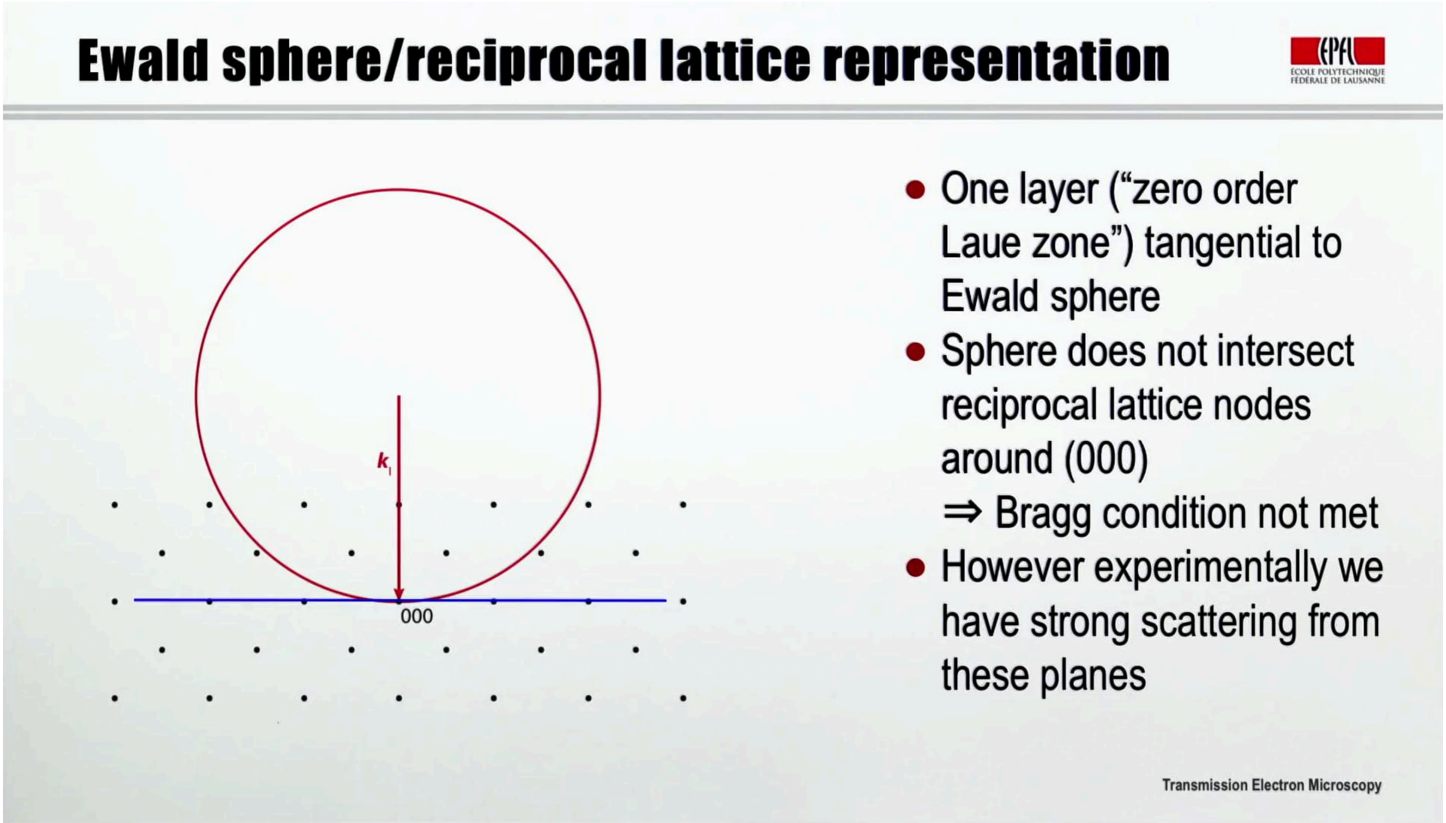


And we can keep on going, and as we do this, we build up this diffraction pattern which, by symmetry, includes inverse planes such as the (–1 0 0) and (0 –1 0). And we can notice a number of things about this. One thing: we can see that it looks like a section through our reciprocal lattice, which indeed it is. Secondly, we have associated each diffraction spot with the Miller indices h k l of the plane that has created it. This is called "indexing the diffraction pattern". The third thing I will point out is that here we have our electron beam parallel to [0 0 1]; so [0 0 1] is our so-called "zone axis". And we can note that all these planes – being parallel to the zone axis – obey the Weiss zone law: h U + k V + l W = 0 – the rule which applies for plane (h k l) being parallel to a lattice vector [U V W].

Notes

Summary

11m 12s

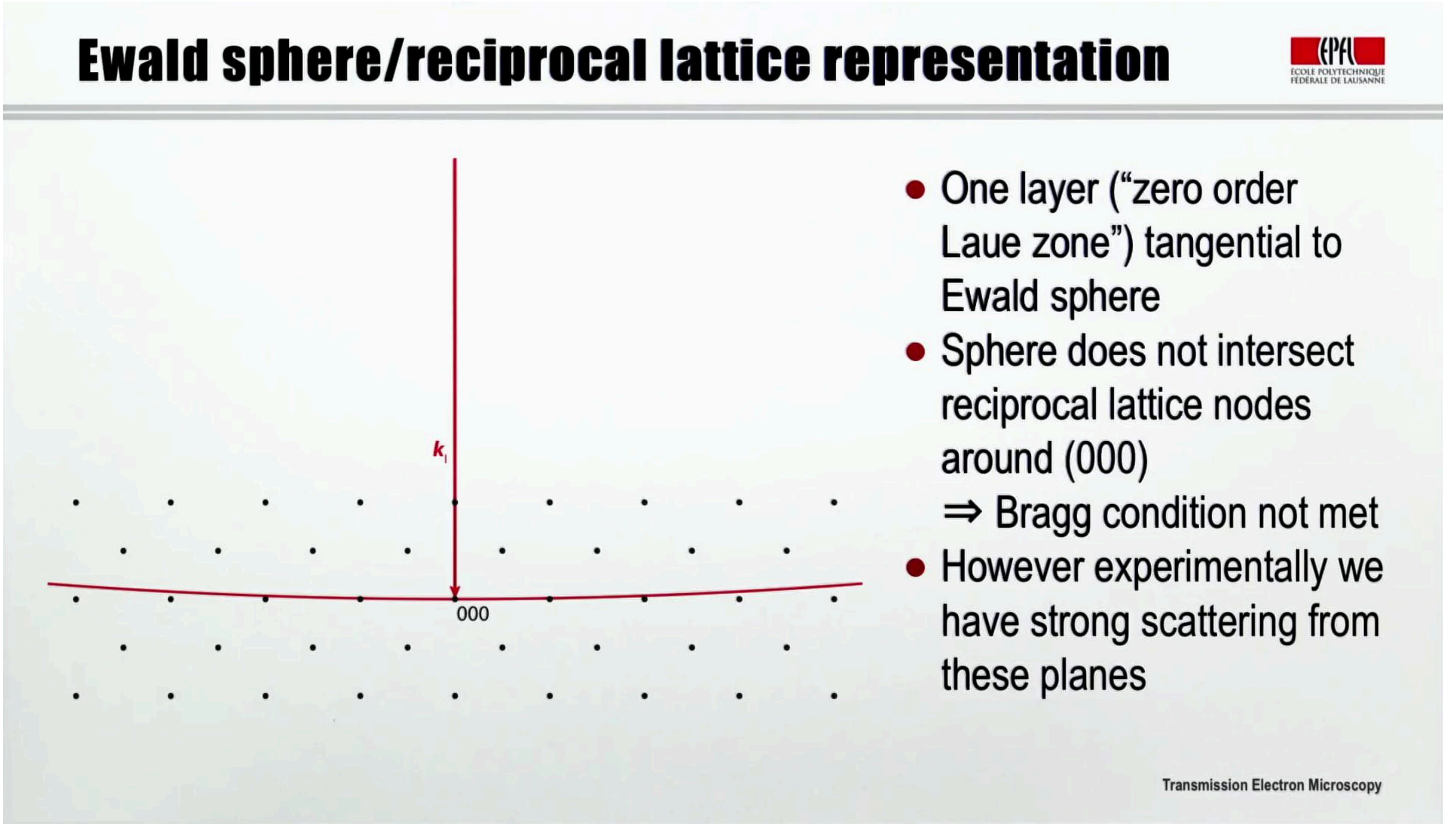


Now we have looked at the formation of the zone axis diffraction pattern by the simple analogy of the crystal as a diffraction grating, we should instead look at the diffraction pattern formation by the Ewald sphere/ reciprocal lattice representation. So that is what I have done here. Here we have the Ewald sphere, and the vector for the incident beam k_I. And, when we have this geometry, what we see is that one layer of this reciprocal lattice is now tangential to the Ewald sphere. And what is more is that, when we have this geometry, we see that the Ewald sphere actually does not intersect any of the reciprocal lattice nodes in this layer directly around the 0 0 0 beam. In other words, the Bragg condition is not met. Now this was the exaggerated Ewald sphere representation that I showed before. We can make it a realistic representation, as follows.

Notes

Summary

12m 19s

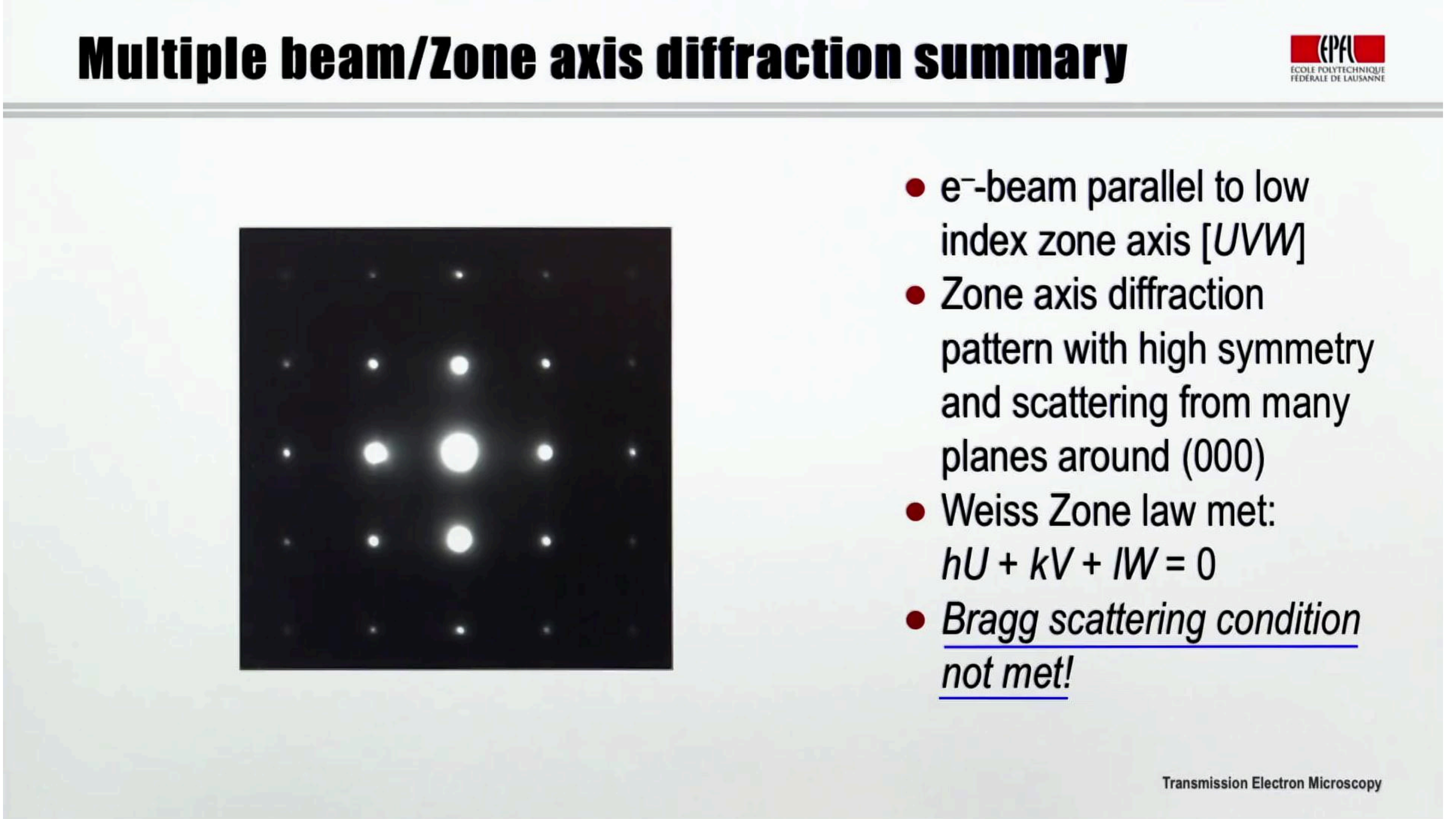


So here, now the curvature of the Ewald sphere corresponds to what we would see for a 200 kilovolt beam, and a reciprocal lattice for body centered cubic iron. But even in this case we can see that, even with this very flat Ewald sphere, the surface of that sphere does not intersect most of these reciprocal lattice nodes. In other words, the Bragg condition of scattering for these reciprocal lattice nodes is not met. And if the Bragg condition is not met, theoretically there should be no scattering from these planes, and we should not have all these diffracted beams that we in fact see. Because experimentally, we know we have strong scattering from many planes in this zone axis condition. So, we have some problem in our representation using the Ewald sphere and reciprocal lattice, for the zone axis condition.

Notes

Summary

13m 26s



To summarize, when the electron beam is parallel to some important crystallographic direction, or so-called low index zone axis [U V W], we obtain a zone axis diffraction pattern which has multiple scattering in many different beams. This pattern can display high symmetry, with mirror and rotational symmetries which correspond to that of the real crystal lattice. Further, in this condition, we had diffraction from planes which are parallel to the incident beam, and so parallel to the zone axis [U V W]. And because of this, the Weiss zone law is met. So all of the planes directly around the direct beam obey the Weiss zone law, where for the plane (h k l): h U + k V + l W = 0 On the other hand, when we represent this condition using our Ewald sphere/reciprocal lattice representation, we find that the Bragg scattering condition is not met. Clearly there is a problem in our representation. The problem in our representation is because, while the reciprocal lattice nodes so far have been represented as infinitely small points, in fact they have a size and a shape – and the size and shape leads to a relaxation of the Bragg scattering condition, and we obtain multiple beam scattering in our schematic diagram. And this is what we will look at in the next lecture.

Notes

Summary

14m 27s