Symmetry and Structure in the Solid State
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Lecture – 45
Systematic Absences 2

(Refer Slide Time: 00:39)

Systematic absences displayed by conventional lattice types

	Coordinates of lattie points	Systematic absence
P	0, 0, 0	None
A	0, 0, 0; 0, $\frac{1}{2}$, $\frac{1}{2}$	$k+l=2n+1$
B	0, 0, 0; $\frac{1}{2}$, 0, $\frac{1}{2}$	$h+l=2n+1$
C	0, 0, 0; $\frac{1}{2}$, $\frac{1}{2}$, 0	$h+k=2n+1$
F	0, 0, 0; 0, $\frac{1}{2}$, $\frac{1}{2}$; $\frac{1}{2}$, 0, $\frac{1}{2}$; $\frac{1}{2}$, $\frac{1}{2}$, 0	h, k, l *neither* all odd *nor* all even
I	0, 0, 0; $\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$	$h+k+l=2n+1$
R (hexagonal axes)	0, 0, 0; $\frac{2}{3}$, $\frac{1}{3}$, $\frac{1}{3}$; $\frac{1}{3}$, $\frac{2}{3}$, $\frac{2}{3}$	$-h+k+l=3n\pm1$
R (rhombohedral axes)	0, 0, 0	None

So, we have been discussing the appearance of systematic absences depending upon the lattice types. And here is a list of all possible lattices in the seven crystal system, which will ensure the number of coordinates and coordinates of the lattice points which are shown here. And the type of systematic absence, we get as a consequence of the centering of the lattice.

So, the primitive lattice obviously, therefore will not have any systematic absences. What it means is that all the primitive lattices, which come in all the seven crystal systems, will not have any systematic absences associated with general reflections. So, if you take reflections h, k, l, all values of h, all values of k, all values of l, then the systematic absences associated with a primitive lattice will be none. In the sense that, in principle all the reflections allowed are present.

Of course, the primitive lattice may carry information about the symmetry, which could be having a translational component like a screw axis or a glide plane, we shall discuss that later on. But, at the moment whenever there is a primitive lattice, and none of no translational component associated with the symmetry elements like for example, *P* 1, and *P* $\bar{1}$, *P* 2, *P* m, and things like *P* 2/*m* and things like that, there will be no systematic absences.

So, systematic absences come up with the centering, so if there is *A* centering, we will have the systematic absence coming in terms of the values which the which adds on to the axis, so whichever axis to which the ½ adds on. Those axis will show the systematic absences. So, we get k + l = to 2n + 1 for the *A* centering, *B* centering h + l is 2 n + 1, and *C* centering h + k is 2 n + 1. We have discussed the appearance and how it influences the expression for the structure factor in earlier classes.

And therefore, right now we will see that for the face centered, which we discussed with the example of Zinc Sulphide, h, k, l neither all odd nor all even that means, they have to be in such a way that all the three indicated here above should be simultaneously satisfied for a reflection to be systematically absent. What is listed in the international table, which we will have a look later on or not the systematic absences, but systematic presences, so that is something which we should remember, when we look at the international tables for reference.

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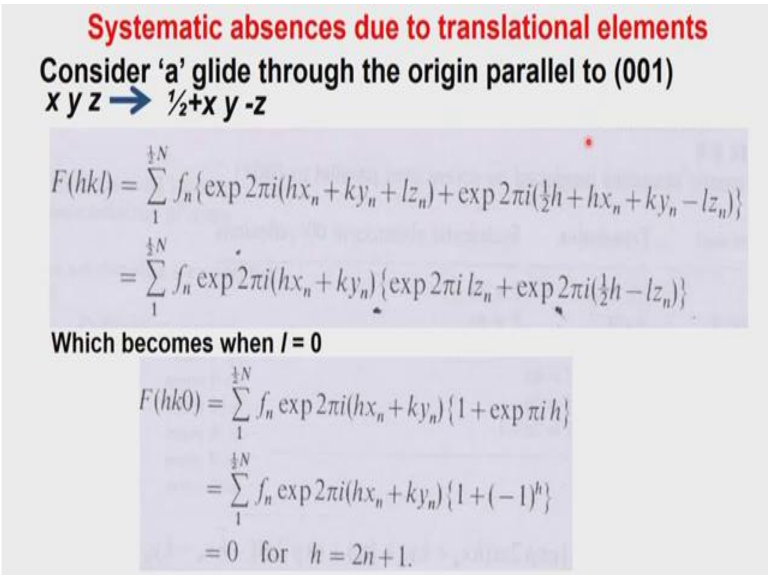

So, having seen this we now go and see, what are the systematic absences, which come due to the presence of translational components in the symmetry associated with the space group? So, the space group the lattice type, we have seen. Now, let us say there is a space group, which is associated with an *a* glide.

Let us take an example of a primitive lattice with an *a* glide, it could be an *I* centered lattice with an *a* glide in a monoclinic system or centering could be also a reason, which is introducing the *a* glide. So, if there is an *a* glide which is now in any of the directions associated with x, y, z. Suppose there is *a* glide which goes through the origin, and is parallel to 0 0 1 the plane 0 0 1 the z-axis.

Then, you see that x, y, z every point x, y, z, we will give rise to a ½ + x y and , so that means the *a* glide operation takes the point x, y, z to ½ + x y . And, if we operate again on this one, the *a* glide will go back to that, so that is the group which we are considering. And what happens to the structure factor expression, so we write the F(h k l) expression as before, it is 1 to N, f_n exp 2πi (h x + k y + l z).

And, we also have due to the second equivalent position, because again these two are equivalent of each other, we separate them into two parts. So, the summation goes from 1 to N/2 and f_n exp 2πi (h x_n + k y_n + l z_n) + exponential 2πi. This is ½ + x, so ½ + h adds on here, {½ h + h x_n + k y_n - l z_n}. And, this can be simplified and written as sum over 1 to ½ of N, f_n exp 2πi (h x_n + k y_n) exponential this quantity + exponential that quantity.

Now, remember in the previous case, when we were discussing the *C* centered lattice, we had expressions of on the other side of the common factor, which involved only exponential to be raised to a integer. In other words, we had expressions of this current exp 2πi (h/2) kind of thing, but we did not have any of the independent axis that is associated with it.

So, therefore, when we have an a glide parallel to 0 0 1, we look at not the general reflection, so there will be no general systemic absence. For example, *P* a if it is a space group, primitive will not give any systematic absence associated with general reflections. But, the *a* glide will give systematic absences, when l is put equal to 0.

What happens, when l is put equal to 0 is this expression will now simplify, so we write the expression for F(h k 0) that means we are now looking at only the projection reflections. We look at different values of h, different values of k, but 0 value for the z value. So, whenever this is 0, it is a projection down the z-axis. And, the expression becomes 1 to ½ of N, f_n exp $2\pi i$ (h x_n + k y_n) * (1 + exp πih).

You see, now what I was mentioning has happened? In this case, we have therefore only the integers in this part of the flower bracket. And, when you have a integers in the part of the as flower bracket, we can calculate mathematically the value, and that turns out to be $1 + (-1)^h$. So, depending on the value of h, this value will be either 2 or 0, so it will be 1 + 1 or 1 + (-1), which is 0 or $1 + (-1)^h$ that will make it -1 or + 1.

And, whenever this is + 1, it will be that h = 2n + 1, that means all odd values of h, this particular value 1 - 1 will cancel out, and therefore this will become 0, and therefore the value becomes 0. So, the systematic absence associated with *a* glide passing through the going is along the z-axis or parallel to the z-axis, *a* is perpendicular to the 0 0 1 plane. Then, it F(h k 0) is 0 for which h odd is absent, so h = 2 n + 1.

So, this therefore that tells us that we can have systematic absences due to glide operations. We have already seen how many glide operations are possible *a* glide, *b* glide, *c* glide, *n* glide, *d* glide in a special situation. So, all these glides, therefore will give rise to systematic absences depending upon the projection reflection. So, it is only the projection reflections, which will show you systematic absences, and we will examine it a little more closely.

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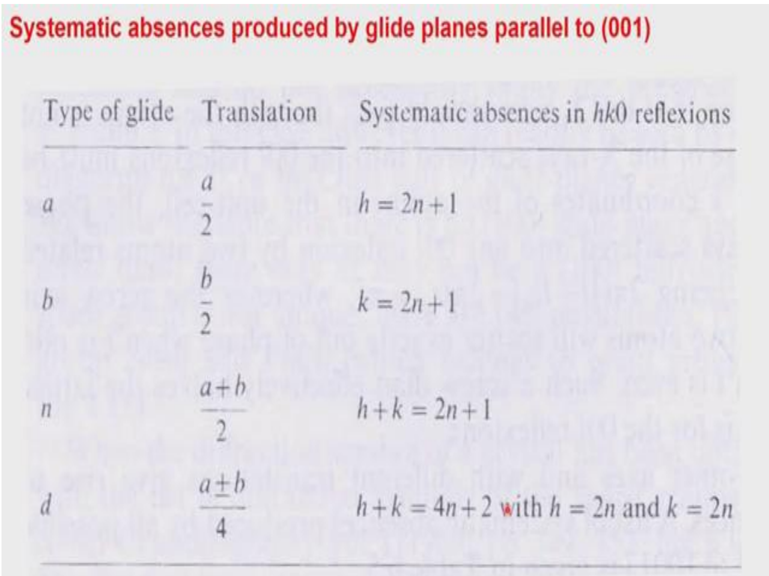

Systematic absences produced by glide planes parallel to (001)

Type of glide	Translation	Systematic absences in *hk*0 reflexions
a	$\frac{a}{2}$	$h = 2n+1$
b	$\frac{b}{2}$	$k = 2n+1$
n	$\frac{a+b}{2}$	$h+k = 2n+1$
d	$\frac{a\pm b}{4}$	$h+k = 4n+2$ with $h = 2n$ and $k = 2n$

Let us take all possible *a* glides. If you have all possible *a* glides the type of glide is *a* glide, then the translation is *a* divided by 2. Whenever *a* is involved, it is h = 2n + 1, which is systematically absent. For the *b* glide, it is *b* by 2; k = 2n + 1. And, of course, we cannot have a *c* glide parallel to 0 0 1, we know that. And therefore, there is no *c* glide associated with the glide planes parallel to 0 0 1.

But, we can have *c* glides parallel to the other two directions that means, two other two planes 0 1 0 and 1 0 0 can have *c* glides. 0 0 1 which is which is a plane, which is associated with the direction of z, it is perpendicular to the direction of z. So, *c* glide is not allowed, because the translation has to be ½ along that particular direction.

So, we have therefore the *a* glide and the *b* glide, we can also invoke the presence of the *n* glide, which is a + b by 2. Then, we will have the systemic absence h + k is 2n + 1. But, all these systematic absences occur in only projection reflections, projection reflections associated with these. So, in this case for example, it is h k 0. In this particular case, what would be the thing, I want you to find out it will be h k 0, but this time the k is equal to 2n + 1. So, the systematic absences are all in h k 0 reflections.

So, in the case of *a* glide, it is a h odd. In the case of *b* glide, it is k odd. In case of the *n* glide, it is h + k odd. And in case there is a diamond glide, which we have not discussed which is probably out of the scope of this course. We will not consider this, but it will also have systematic absences as shown below it is just for our record, we are not going to discuss how it turns out.

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Symmetry elements		Set of reflections	Conditions
Glide-plane ǁ (100)	*b*	0*kl*	$k = 2n$
	c		$l = 2n$
	n		$k + l = 2n$
	d		$k + l = 4n$
Glide-plane ǁ (010)	*a*	*h*0*l*	$h = 2n$
	c		$l = 2n$
	n		$h + l = 2n$
	d		$h + l = 4n$
Glide-plane ǁ (110)	*c*	*hhl*	$l = 2n$
	b		$h = 2n$
	n		$h + l = 2n$
	d		$2h + l = 4n$

So, if that is the case, what are the types of glide planes, we can think of, we can think of glide planes parallel to 1 0 0 direction, which is along the *a* axis. Glide plane parallel to 0 1 0, which means its *b*, and glide planes parallel to 1 1 0, which is which is along the diagonal.

So, we have listed therefore the planes, which are in these directions, and the glide planes which are along 1 0 0 can be *b, c, n* and *d*. 0 1 0 is *a, c, n, d* of course, we can always have 0 0 1 which we already discussed, so we have not put it here. And, the glide plane 1 1 0, it can be *c, b, n* and *d*. And, the set of reflections that will get affected in the case of the glide plane, parallel to the plane 1 0 0 is 0 k l glide plane associated with 0 1 0 is h 0 l and glide plane this will be h h l.

And, so the systematic absences are listed here. And, these will be the condition, here you see on the right side, we did not list the systematic absences, but we have listed the systematic presences. So, k even only present, l even only present in the example of a glide plane, which is which has a *b* glide, and *c* glide respectively it is k = 2n, l = 2n.

So, the conditions for getting the reflections measurable are given here, and this is what you will see in the international tables. But, for the discussion sake which we have done so far, the lattice centering, and then also the *a* glide which is which we have discussed in detail. We have discussed the systematic absences, because it is always good to see what is absent than what is present, I mean that is normally the logic you know the there is a statement that if in an audience in the classroom for example, if all students are present, their presence will be ignored. Those who are absent, they will be noted. So, it is something like that.

So, systematic absences therefore are very crucial to notice, and that is why systematic absences are discussed before. But, what is present is more important from the point of view of the diffraction condition, and therefore the presences are listed here. So, international tables for crystallography will list only the systematic presences, what are present systematically alright.

So, this is as far as the presence of the glide plane is concerned. So, we have seen the lattice centering, and now we have seen the glide planes. So, glide plane give systematic absences associated with projection reflections. The general reflection systematic absence give the lattice centering information.

So, the next obvious choice is the presence of the screw axis. So, what is the plane that it can affect, it can affect not the planes, but axial reflections. By axial reflections, I mean it will affect the h 0 0, k 0 0, and the l 0 0 with respect to hkl plane. So, it is therefore, the actual reflections that define the h direction, the k direction, and the l direction, h = 1, 2, 3, 4 like that.

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Systematic absences produced by screw axes parallel to [001]

x y z → -x -y ½+z

$$F(hkl) = \sum_{1}^{\frac{1}{2}N} f_n\{\exp 2\pi i(hx_n + ky_n + lz_n) + \exp 2\pi i(-hx_n - ky_n + \tfrac{1}{2}l + lz_n)\}$$

$$= \sum_{1}^{\frac{1}{2}N} f_n \exp 2\pi i\, lz_n\{\exp 2\pi i(hx_n + ky_n) + \exp 2\pi i(-hx_n - ky_n + \tfrac{1}{2}l)\}$$

which becomes when $h = k = 0$,

$$F(00l) = \sum_{1}^{\frac{1}{2}N} f_n \exp 2\pi i\, lz_n\{1 + \exp \pi i\, l\}$$

$$= \sum_{1}^{\frac{1}{2}N} f_n \exp 2\pi i\, lz_n\{1 + (-1)^l\}$$

$$= 0 \quad \text{for} \quad l = 2n+1$$

So, what happens in such a situation is again, we have to write the general expression for the structure factor. And, then evaluate the structure factor features associated with it let us let us look at it in a careful manner. So, in this case the systematic absence, we now consider produced by screw axis. Please notice the nomenclature; I am just reminding you that when we put in square bracket, it represents the direction.

When we put in ordinary brackets, it represents the plane. So, the previous representation was with respect to the plane, and this is now with respect to the direction, so this is along the z-direction. So, when we talk about the screw axis, the screw axis or parallel to the 0 0 1. And, when we talk about the glide planes and we have written parallel to that in the parallel to the planes 1 0 0, 0 0 1, and 0 1 0.

So, systematic absences produced by screw axis now the direction is 0 0 1. So, x, y, z, now will become , , and you see since the translation component is along the z direction, we have ½ + z in that direction. So, this screw operation, again operated will take you back to x, y, z defining the point group.

So, whenever you have a crystal system like $P\ 2_1$ for example, a primitive lattice with 2_1. Then you will have this systematic absence coming up, how it comes up, we will discuss in a minute. So, again we write the general expression for F(h k l), you see again we have to consider ½ the number of total reflections, because one ½ will obey this, the other ½ will obey that. And, so the expression now f_n {exp $2\pi i$ (h x_n + k y_n + l z_n) + exp $2\pi i$ (-h x_n - k y_n + ½ l + l z_n)

So, we now take out the common factor, and rewrite this expression the common factor here between these two is exp $2\pi i$ (l z_n) f_n. So, this therefore becomes 1 to ½ of N, f_n exp $2\pi i$ (l z_n), and exp $2\pi i$ (h x_n + k y_n) as far as this first expression is concerned. And, as far as the second expression is concerned, it is (-h x_n - k y_n + ½ l).

So, the same logic as we defined in the previous case that we would like to have a expression which will essentially depend upon integral values to take the exponential, then we can calculate it mathematically, and so we separate it out. The way to separate it out is to put h = and k = both equal to 0.

So, if h and k are both equal to 0, we have only reflections of the type 0 0 l. So, these F(0 0 l) now will be having a formula reduction, which is going from 1 to ½ of N, f_n exp $2\pi i$

($l\ z_n$), multiplied by this since h is 0, k is 0, this will go. And, therefore, you get ($1 + \exp \pi il$). And, we know this value can be $(-1)^l$. And therefore, it has to be again the same logic that whenever l is odd, F(0 0 l) will be absent. So, the systematic absences associated with the with the screw axis essentially affects only the axial reflections, so, the reflections which go along the definition of the axis either h or k or l.

(Refer Slide Time: 17:45)

Systematic absences produced by screw axes parallel to [001]

Screw axis	Translation	Systematic absences in 00*l* reflexions
2_1	$c/2$	$l = 2n+1$
4_1 and 4_3	$\pm c/4$	$l \neq 4n$
4_2	$c/2$	$l = 2n+1$
3_1 and 3_2	$\pm c/3$	$l \neq 3n$
6_1 and 6_5	$\pm c/6$	$l \neq 6n$
6_2 and 6_4	$\pm c/3$	$l \neq 3n$
6_3	$c/2$	$l = 2n+1$

And, so we can now write down those expressions, and see how it comes about. So, we can have screw axis in variety of crystal systems as we know, we can have 2_1 screw, we can have a 4_1, 4_3, 4_2 in a tetragonal system. We can have 3_1 and 3_2 in a trigonal system. We can have 6_1, 6_5, 6_2, 6_4, 6_3 in an hexagonal system. So, these are all the possible screw axis, we can have in a crystal system.

And therefore, we now look at the corresponding systematic absences. If, the screw axis is parallel to the z direction, so that will affect the 0 0 l reflections only, and the condition is on l value. And, that condition on l value for 2_1 screw axis, the translation is along the z direction. So, it it moves along the *c* axis, *c* divided by 2, that is the translation associated with the screw axis.

So, we get therefore the systematic absences to be l = odd, so all odd reflections will be absent. What is interesting is the systematic absences follow a certain trend among the tetragonal, and the trigonal, and the hexagonal systems that is because in all these cases the unique axis is z. And therefore, the screw axis is parallel now to the unique axis.

Since, the screw axis is parallel to the unique axis or along the unique axis, the systematic absences will develop differently depending upon the nature of the screw axis operation which we invoke. For example, if you have a 4_2 axis, for all practical purposes a 4_2 axis is effectively a 2_1 axis, and therefore you will have only l odd absent.

So, suppose there is a space group $P\ 4_2$, then the systematic absence in that particular space group will be just 0 0 l, l odd absent. On the other hand if you have a screw axis 4_1 and 4_3, these two axis are now in two opposite directions, but representing the same effective positioning of the atoms except that the handedness of associated with 1 and 3 will change.

And therefore, l is going to be $\neq$ 4n that means, whenever l = 4n, you will get the reflection. So, n can be equal to 1, so you get reflections like 4, 8, 12 and so on. Multiples of n, n can take values 1, 2, 3, 4 etc.., So, it depends upon the length of the unit cell, suppose the unit cell length is about 20, then you will have the reflections coming only for those reflections 0 0 l which is l = 4, l = 8, l = 12, l = 16, and l = 20. So, you will get five reflections along the axial line.

So, you can easily observe, when you look at the reciprocal lattice image, which you have measured. And, particularly if you have done a photographic measurement, it is easily seen in earlier days. But, now a days you can always have a program which looks into the possible systematic absences, when once you have a collection of all the hkl reflections. So, you have done the experiment, you have put the crystal on the beam, you get the diffraction done.

And, then you have the reciprocal lattice image, the images of the reciprocal lattice, you examine, after indexing them with respect to h, k, and l. We will see how that is done in a after probably in a couple of classes, we will know it the authoritatively how to do that. And, when once we have this hkl information available to us, we examine the values of hkl, and the systematic absences will show, if there is anything.

For example, in this case all values of l = 4n will be present. So, we can easily identify as far as 0 0 l is concerned, whether it is 4_1, and 4_3, for both it is the same systematic absence. Same is true with 3_1 axis, and the 6_1, and 6_5, you see l $\neq$ 3n, l $\neq$ 6n. And, in case of 6_2, 6_4 also, it is l $\neq$ 3 n.

So, what it means is that if we by looking at the systematic absences associated with these crystal systems, you cannot decide the space group, please note the point. Suppose, there is a space group, which is *P* 3_1, and then a crystal system which goes into *P* 3_2, by just looking at the systematic absences, you cannot say whether it is 3_1 or 3_2. Same is true with 6_1, 6_5; same is true with 6_2, 6_4; and same is true with 4_1, 4_3.

So, only when you have the ½ the translation of the length, for example 6_3, for example a 4_2, because there is no ½ translation possible in the threefold-axis. So, $3/6^{th}$ is one effectively, if you divide this by 3, it will become 2_1, 4_2, we divide by 2, it will become 2_1 and 2_1. So, the systematic absences are all identical, their $l = 2n + 1$.

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Symmetry elements		Set of reflections	Conditions
Screw-axis ∥ *a*	$2_1, 4_2$ $4_1, 4_3$	*h*00	$h = 2n$ $h = 4n$
Screw-axis ∥ *b*	$2_1, 4_2$ $4_1, 4_3$	0*k*0	$k = 2n$ $k = 4n$
Screw-axis ∥ [110]	2_1	*hh*0	$h = 2n$

So, having seen this, we will see what happens in case the systemic and screw axis are in different directions. So, screw axis is parallel to *a*, screw axis is parallel to *b*, and screw axis is parallel to 1 1 0. Whenever the screw axis is parallel to that direction that particular direction only is affected that means h 0 0, h = 2n, and h = 4n are present in these four crystal systems. In these four crystal systems, if the screw axis is *b*, we will see 0 k 0 k = even or k = 4n systematically present. So, these are the present conditions, this is what we mean by conditions, in fact that is what is written in the international tables as well.

Screw axis parallel to 1 1 0 that is quite possible, and then you have therefore the systematic absences h h 0, this is possible in tetragonal systems, because you have a = b in a tetragonal system. So, you can have a 2_1 screw axis, parallel to 1 1 0 direction. Since, the crystal systems could be ideally identified based on these systematic absences.

So, essentially we have now covered all the symmetry elements, which will have translational components. The centering information that is with associated with a lattice will also give ½ ½ additions and so on. And therefore, we have these systematic absences. We have systematic absences due to the glide planes; we also have systematic absences due to screw axis.

So, these translation components which are present only in crystals, you see that is a very important point to remember. These systematic absences are present only in crystals, and they affect only diffraction. And therefore, they it allows for a unique determination in most cases of the space group, just to give you an example. Suppose, there is a space group $P\ 2_1/c$, you for the primitive you get no systematic absences. So, you will have all h k l reflections present in principle. It is not necessary that all hkl value should be measurable, some of maybe weak; some of them may be strong.

And, we know when it is weak, when it is strong by our previous discussions. It depends upon where the atoms are sitting in the unit cell, the contribution to the diffraction, the intensity contribution to the diffraction is coming from individual atoms, which are inside the unit cell, but the measurement which we do is with respect to the plane.

So, what is it that is coming out from the plane? And therefore, we draw we consider this formula D_{hkl}/d_{hkl}. And calculate the values that come to the intensities based upon 2π (h x + k y + l z), and therefore we have this general formula which will allow us to calculate the intensity.

So, the intensities need not be present for all possible hkl, some of them may be absent, some of them may be present. Some of them may be absent, because the waves coming out successively interfere such that they destructively interfere ok. So, when they destructively interfere, we will not get any intensity, it is not a systematic absence. The systematic absence should be throughout the data, what I mean to say is watch my words carefully. If h k l, h + k odd is absent, it will definitely tell you that it is a centered lattice. But, by chance in a general h k l data, some h + k odd may be absent, but it is not systematic that is allowed, then it is still a primitive lattice.

So, only when all the reflections of your h k l collected obey these conditions, then only you can say this has a symmetry. This case becomes very very crucial. In case you have a monoclinic system for example, in case of a monoclinic system, it may so happen you are looking let us say at the unique axis *b*, and it may so happen the unique axis is about 4 Å. You may have *a* and *b* very large, but the *c* axis is 4 Å.

So, if there is a 2_1 screw axis associated with the *b* direction, then what would be the systematic absences, the systematic absences will ensure that only 2 0 0, and 4 0 0 sorry 0 2 0 and 0 4 0 will be present. So, 0 1 0 and 0 3 0 will be absent that is the extent to which we can go, because we can measure only two reflections. In fact, we can measure four reflections 0 1 0, 0 2 0, 0 3 0, 0 4 0. So, we have four reflections at our disposal along the *c* direction, along the *b* direction sorry correction along the unique axis *b*. So, there are four reflections 0 1 0, 0 2 0, 0 3 0, 0 4 0.

So, if they are to be systematically absent, and give rise to the presence of a 2_1 screw axis, we have to measure we should be measuring only 0 2 0 and 0 4 0, they should come with some intensity. It may so happen the the atoms and the molecules inside the crystal may so arrange themselves that 0 2 0 and 0 4 0 may also become very very weak, so weak that we cannot measure them.

Then you will see all the four being absent or in the case of a system which has no screw axis, you may measure let us say 0 2 0, 0 4 0 as possible reflections. It may so happen the atoms again arrange themselves, even though there is no 2_1 screw axis, such that the contribution to 0 1 0 and 0 3 0 is very very small, then it looks as though there is a systematic absence. So, these are all pitfalls in uniquely determining the space group.

So, determination of *P* 2_1 with a unique axis *b* very small is a question. And in such situations, we might have to look at the structure determination. And, when once we determine the structure, in fact determine the structure in both space groups *P* 2 as well as *P* 2_1, and then decide which is the space group into which it goes into.

So, the determination of the structure then becomes crucial to identify the presence of the 2_1 screw axis, so that is where we have to be a little cautious. But, routinely if you have got a *P* $2_1/c$, it will have 2 systematic absences 0 k 0, k odd absent, and h o l, l odd absent. If h o l shows a h + l odd absence, then it will be an *n* glide. So, we can uniquely determine the space group *P* $2_1/c$ or *P* $2_1/n$, by just looking at the systematic absences.

As I said primitive will not give any systematic absence, so you will have all general reflections present. Then you look at the projection reflection. So, systematically you take the data; arrange it in such a way that you have all the general h k l, the projection reflections and then the axial reflections.

And, the projection reflections if you look at now, they will have systematic absences corresponding to the *c* glide that means, h o l, l odd absent. So, the glide planes will affect the projection of the along the plane that means, it is 0 along that particular direction where the axis is located that means, if you have in the case of a monoclinic system, we have a 2_1 and *c*, the unique axis is *b*. So, about the unique axis, we have the 2_1 screw, so 0 k 0, k odd. And about the unique axis, we have the mirror plane perpendicular to that, because the point group symmetry is 2/*m* for $P\ 2_1/c$.

So, we therefore have the systematic absence coming with respect to h o l, l odd absent. So, space groups like $P\ 2_1/c$ can be uniquely determined. And, this is an advantage we have, because this particular feature will enable us to identify the space groups uniquely. So, for a simple discussion many space groups belonging to different crystal systems can be uniquely identified by an examination of the h k l reflections. It is only those in which there is no translational component involved, these space groups are not identified by systematic absences.

So, those space groups of course have to be identified, whether they belong to they belong to the system. And, what is the for example, what are the symmetry elements that are associated with it. Take for example, *P* 2 and *P m*; it is very hard to distinguish between *P* 2 and *P m*, because we do not have systematic absences.

So, of course there are ways and means in which we can identify probably one of the space group to be correct, we will discuss that later, when we look at the intensity scale statistics. So, since intensities come from the scattering overall of the unit cell, so it does not matter in principle to the intensity the orientation of the planes. The intensity is coming from the electron density, and the electron density is continuous in the space.

So, the way the intensities distribute themselves among various let us say values of $\sin\theta$ / λ, because we know that is the one which controls it, because scattering factor falls off with respect to $\sin\theta$ / λ asymptotically. So, since scattering factor falls off with respect to $\sin\theta$ / λ asymptotically, we have a dependence of the intensity on that value of that particular atom. And, so the intensities will fall off with respect to $\sin\theta / \lambda$. Apart from that the intensity is therefore distribute themselves into various regions of the scattering angle, so there is a statistical evaluation that is possible for the intensities.

It so happens, for example if you have a space group P 1 and space group $P\ \bar{1}$, the distinction between P 1 and $P\ \bar{1}$ is fairly straightforward in the context of intensity statistics. Because, the intensity distribution will be different in case of 1 compared to the distribution in case of $\bar{1}$. And this we will discuss when we do the scaling operation and how to put the intensities on an absolute scale. At that time we will discuss this issue, because that is it is at that time we can distinguish in such cases, where systematic absences are not available, we have to find out the nature of the space group.

So, whether P 1 and $P\ \bar{1}$ there is a triclinic system, whether the crystals are now going into a centric system or a non-centrosymmetric system can be identified only by an analysis of the intensity statistics, which goes along with it. So, to summarize all the issues done so far, we have identified systematic absences with respect to the lattice centering. So, we have identified systematic absences with respect to the glide planes to be with those of projection reflections, and with the screw axis with those of axial reflections.

So, once we accumulate a data, collect the data, after doing the diffraction experiment. We need to analyze the h k l reflections, for this systematic presence or absence. And, if this is nicely satisfied, we can uniquely determine the space group. If, it is not nicely satisfied, we can still have an ambiguity in the space group. We can still identify the space group, but we can say this is this or that.

For example, we discussed just now the possibility of 3_1 and 3_2, so we can say well the space group is $P\ 3_1$ or $P\ 3_2$, but we are not sure whether it is 3_1 or 3_2 as of now. And, that those are in fact 3_1 and 3_2 are known as an enantiomorphous space groups. And it is required to do the structure in both, and finally identify which is the realistic space group associated with 3_1 and 3_2.