

Crystals, Symmetry and Tensors
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Lecture 21 b
3D Point Groups XV: Laue Classes

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3D Point Groups XV : Laue Classes

Point Group of a Crystal

Point Group of the Diffraction Pattern of the Crystal

Friedel's Law

Point Group of the Diffraction Pattern \neq Point Group of the Crystal

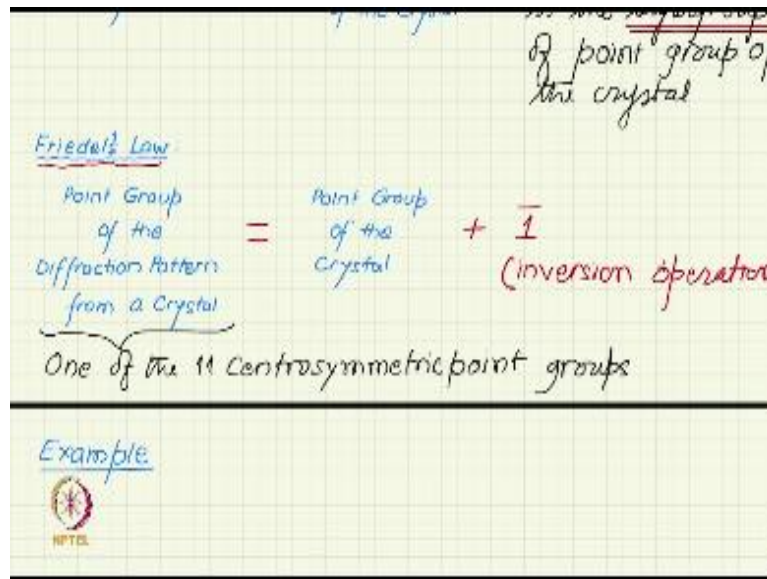
3D Point Groups XV : Laue Classes

Point Group of a Crystal \neq Point Group of the Diffraction Pattern of the Crystal

Neumann's Principle
 Point group of a physical property is the supergroup of point group of the crystal

Friedel's Law

Point Group of the Diffraction Pattern $=$ Point Group of the Crystal $+ \bar{1}$
 (inversion operation)



So, in this video we will discuss what is an important concept known as Laue classes, Laue classes. So, in the last video of this series we discussed the so-called centrosymmetric point groups and Laue classes are related to the centrosymmetric point group. The question the larvae classes relates to what is the symmetry of diffraction pattern?

So, a crystal has a particular point group which is the point group of the crystal because of the symmetry of the crystal diffraction pattern will also show a symmetry and we can say the diffraction pattern also has its own point group.

The question is, is the point group of the diffraction pattern exactly the same as point group of a crystal or not? Means as a first approximation or intuitively we will feel that the symmetry of the diffraction pattern should be the same as symmetry of the point group.

But it turns out that it is not actually the same the two are not equal and in fact this inequality is true not only for diffraction pattern but for many physical properties of the crystal and its described by a principle called Neumann's Principle. Which says point group of a physical property, property is the super group of point group of the crystal. But by super group here we mean that the point group of the physical property will contain all the symmetry of point group of the crystal but it can have more.

The same thing is true for diffraction pattern also diffraction pattern will have all the symmetry of the point group of a crystal but it can have more. And there is another law called Friedel's Law which actually tells what is that more and that shows us that point group of the diffraction pattern of a crystal is buoyant group of a crystal plus a center of inversion.

Center of inversion will automatically get added in the symmetry of the diffraction pattern. 1 bar Center of inversion or an inversion operation you can say instead of writing center of inversion you can write inversion operation. You add an inversion operation to the point group of the crystal you will get point group of the diffraction pattern.

Because of this you really, let us see an example, so because of this so while developing the centrosymmetric that is why the centrosymmetric point group so the diffraction pattern will always be centrosymmetric point group.

Because of this one bar addition point group of the diffraction pattern will be one of the one of the 11 centrosymmetric point groups which we discussed in the last video. So, the crystal can have any of the 32 point groups but the diffraction pattern will have only one of these 11 centrosymmetric point groups.

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One of the 11 Centrosymmetric point groups

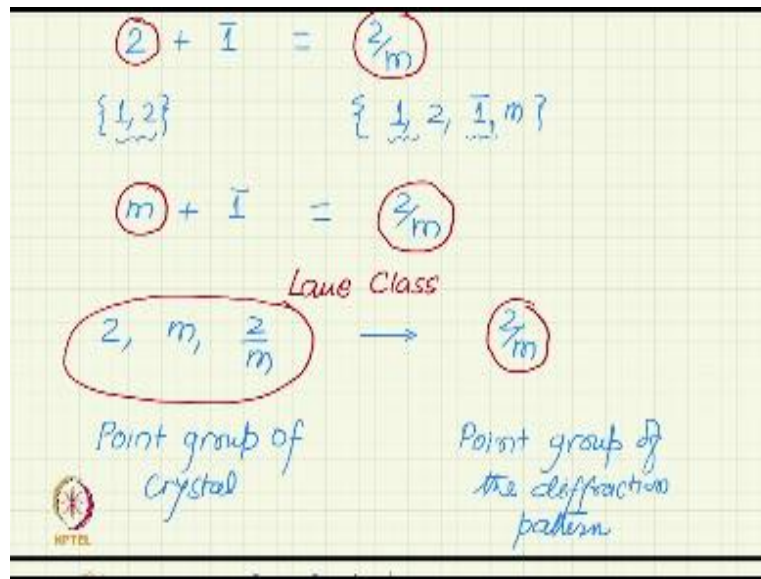
Example

$$\textcircled{2} + \bar{1} = \textcircled{2/m}$$

$$\{\underline{1}, \underline{2}\} \quad \{\underline{1}, \underline{2}, \underline{\bar{1}}, \underline{m}\}$$

$$\textcircled{m} + \bar{1} = \textcircled{2/m}$$

$\textcircled{2}, m, \frac{2}{m}$



So, let us look at an example. So, when developing the central symmetric point group we already saw that if the starting point group is 1 and if we add a center of inversion then we get a point group which is 2 by m.

This this addition has to be interpreted carefully means you are not adding just and 1 bar operation or 1 bar group. So, essentially what you are doing is that the group 2 is a group of order to 1 and 2 and 1 bar is an operation which you want to add to this.

So, the resulting group will be 1, 2 and 1 bar but that will not be enough to complete the group because group should satisfy the closure property. So, this 1 bar operation will combine with both the operation 1 and 2.

So, if it combines with 1 you get 1 bar but if it combines with 2 as you know 2 combined with 1 bar is a 2 bar which is a mirror plane. And that is the mirror plane which is perpendicular to the 2 fold axis and that is why the point group is 2 by m.

We saw it stereographically in the last video. Now, towards the end of the last video we also showed that if you add 1 bar to m again you get 2 by m. Which means by diffraction pattern of a crystal having point group 2 will be 2 by m. Diffraction pattern of a crystal having point group m will be 2 by m and of course a diffraction pattern of a crystal having 2 by m point group will also be 2 by m.

So, which means the point groups 2 m and 2 by m, all of them. So, this is the point group of the crystal all of them will give you a diffraction symmetry which is 2 by m. So, by a simple diffraction experiment we will not be able to distinguish between these two point these three point groups.

We will always get the symmetry 2 by m. So, this is the reason to consider all these three groups into 1 class called Laue Class named after the famous scientist Laue who was the first one to show that diffraction happens from crystals diffract x-rays.

And thus, started the field of x-ray crystallography. So, the three point groups belong to a Laue Class and the Laue Class will be represented by the point group 2 by m.

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Laue Class

$2, m, \frac{2}{m}$

Point group of crystal

→

$\frac{2}{m}$

Point group of the diffraction pattern

| Point Groups belonging to a Laue Class | | | | Laue Class |
|--|---|---|---------------|---------------|
| Triclinic | 1 | 1 | 1 | $\bar{1}$ |
| Monoclinic | 2 | m | $\frac{2}{m}$ | $\frac{2}{m}$ |

| Point Groups belonging to a Laue Class | | | | Laue Class |
|--|-----|-----------|----------------|-----------------|
| Triclinic | 1 | 1 | 1 | $\bar{1}$ |
| Monoclinic | 2 | m | $\frac{2}{m}$ | $\frac{2}{m}$ |
| Orthorhombic | 222 | mm2 | m2m | mmm |
| Tetragonal | 4 | $\bar{4}$ | $\frac{4}{m}$ | $\frac{4}{m}$ |
| | 422 | 4mm | $\frac{4}{m}2$ | $\frac{4}{m}mm$ |
| Trigonal | 3 | $\bar{3}$ | | $\bar{3}$ |
| | 32 | 3m | $\bar{3}m$ | $\bar{3}m$ |
| Hexagonal | 6 | $\bar{6}$ | $\frac{6}{m}$ | $\frac{6}{m}$ |

| | | | | |
|--------------|-----|-------------|-----------------|-----------------|
| Triclinic | 1 | 1 | 1 | 1 |
| Monoclinic | 2 | m | 2/m | 2/m |
| Orthorhombic | 222 | mm2 | mmm | mmm |
| Tetragonal | 4 | $\bar{4}$ | $4/m$ | $4/m$ |
| | 422 | 4mm | $\bar{4}m2$ | $\frac{4}{m}mm$ |
| Trigonal | 3 | $\bar{3}$ | | $\bar{3}$ |
| | 32 | 3m | $\bar{3}m$ | $\bar{3}m$ |
| Hexagonal | 6 | $\bar{6}$ | $6/m$ | $6/m$ |
| | 622 | 6mm | $\bar{6}m2$ | $\frac{6}{m}mm$ |
| | | | $\frac{6}{m}mm$ | $\frac{6}{m}mm$ |
| Cubic | 23 | $m\bar{3}$ | | $m\bar{3}$ |
| | 482 | $\bar{4}3m$ | $m\bar{3}m$ | $m\bar{3}m$ |

So, let us look at this, now for if we carry on this exercise for all the point groups. So, if you add inversion center to 1 it becomes 1 bar. 1 bar already has an inversion center, so you get 1 and 1 bar as one Laue Class which belongs to the Triclinic Crystal System. Similarly, 2 m and 2 by m we just saw belongs to the Laue Class 2 by m. In the Orthorhombic 222 mm2 and mmm if I add center of inversion to any of these it will become mmm. So, they belong to a single Laue Class mmm.

In the Tetragonal point group in the Tetragonal Crystal System there are 7 point groups there are 7 point groups. But they belong to 2 different Laue classes $4\bar{4}$ bar and 4 by m belong to 1 law of a class 4 by m and 422 4mm $4\bar{4}$ bar m2 and 4 by mmm. They represent another Laue Class 4 by m mm.

Similarly, in the Trigonal also we have two Laue classes represented by $3\bar{3}$ bar and $3\bar{3}$ bar m. In Hexagonal 2 Laue classes 6 by m and 6 by m mm. So, the Laue Class 6 by mmm has 4 point groups shown here.

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| Crystal System | Point Groups | Laué Class |
|----------------|---|-----------------|
| Orthorhombic | 222, mm2, mmm | mmm |
| Tetragonal | 4, $\bar{4}$, $\frac{4}{m}$ | $\frac{4}{m}$ |
| | 422, 4mm, $\bar{4}m2$, $\frac{4}{m}mm$ | $\frac{4}{m}mm$ |
| Trigonal | 3, $\bar{3}$ | $\bar{3}$ |
| | 32, 3m, $\bar{3}m$ | $\bar{3}m$ |
| Hexagonal | 6, $\bar{6}$, $\frac{6}{m}$ | $\frac{6}{m}$ |
| | 622, 6mm, $\bar{6}m2$, $\frac{6}{m}mm$ | $\frac{6}{m}mm$ |
| Cubic | 23, $m\bar{3}$ | $m\bar{3}$ |
| | 482, $\bar{4}3m$, $m\bar{3}m$ | $m\bar{3}m$ |

| Crystal System | Point Groups belonging to a Laué Class | Laué Class |
|----------------|--|------------|
| Triclinic | C_1 , C_2 | C_1 |

| Crystal System | Point Groups belonging to a Laué Class | Laué Class |
|----------------|---|-----------------|
| Triclinic | 1, $\bar{1}$ | $\bar{1}$ |
| Monoclinic | 2, m, $\frac{2}{m}$ | $\frac{2}{m}$ |
| Orthorhombic | 222, mm2, mmm | mmm |
| Tetragonal | 4, $\bar{4}$, $\frac{4}{m}$ | $\frac{4}{m}$ |
| | 422, 4mm, $\bar{4}m2$, $\frac{4}{m}mm$ | $\frac{4}{m}mm$ |
| Trigonal | 3, $\bar{3}$ | $\bar{3}$ |
| | 32, 3m, $\bar{3}m$ | $\bar{3}m$ |
| Hexagonal | 6, $\bar{6}$, $\frac{6}{m}$ | $\frac{6}{m}$ |
| | 622, 6mm, $\bar{6}m2$, $\frac{6}{m}mm$ | $\frac{6}{m}mm$ |
| Cubic | 23, $m\bar{3}$ | $m\bar{3}$ |
| | 482, $\bar{4}3m$, $m\bar{3}m$ | $m\bar{3}m$ |

| Crystal System | Point Groups belonging to a Laué Class | Laué Class |
|----------------|---|-----------------|
| Triclinic | 1, $\bar{1}$ | $\bar{1}$ |
| Monoclinic | 2, m, $\frac{2}{m}$ | $\frac{2}{m}$ |
| Orthorhombic | 222, mm2, mmm | mmm |
| Tetragonal | 4, $\bar{4}$, $\frac{4}{m}$ | $\frac{4}{m}$ |
| | 422, 4mm, $\bar{4}m2$, $\frac{4}{m}mm$ | $\frac{4}{m}mm$ |
| Trigonal | 3, $\bar{3}$ | $\bar{3}$ |
| | 32, 3m, $\bar{3}m$ | $\bar{3}m$ |
| Hexagonal | 6, $\bar{6}$, $\frac{6}{m}$ | $\frac{6}{m}$ |
| | 622, 6mm, $\bar{6}m2$, $\frac{6}{m}mm$ | $\frac{6}{m}mm$ |
| Cubic | 23, $m\bar{3}$ | $m\bar{3}$ |
| | 482, $\bar{4}3m$, $m\bar{3}m$ | $m\bar{3}m$ |

In the Cubic crystal system, we have again 2 Laue classes 23 and $m\bar{3}m$ belong to $m\bar{3}m$ and the other three 432 , $4\bar{3}2$, $3m$ and $m\bar{3}m$ belongs to another Laue class.

So, if you see here these are the 11 centrosymmetric point groups and they represent 11 Laue classes. All 32 point groups belong to the 7 crystal systems shown here. When added when a center of symmetry is added will fall into one of these Laue classes. So, that is the idea of Laue class.

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| Laue Classes in Schoenflies notation | Point Groups belonging to a Laue Class | Laue Class |
|--------------------------------------|---|----------------------|
| Triclinic | C_1 C_i | C_1 |
| Monoclinic | C_2 C_s C_{2h} | $2/m$ |
| Orthorhombic | D_2 C_{2v} D_{2h} | D_{2h} |
| Tetragonal | C_4 S_4 C_{4h} D_4 C_{4v} D_{2d} D_{4h} | C_{4h} D_{4h} |
| Trigonal | C_3 C_{3i} D_3 C_{3v} D_{3d} | C_{3i} D_{3d} |
| Hexagonal | C_6 C_{3h} C_{6h} D_6 C_{6v} D_{3h} D_{6h} | C_{6h} D_{6h} |
| Cubic | T T_h O T_d O_h | T_h O_h |

Just to complete the discussion I just show the same table which I showed you above in show and flies notation. So, here showing flies notation is used to describe all the point groups and the corresponding 11 laue classes. Thank you very much.