Symmetry and Structure in the Solid State

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Lecture – 01
Symmetry in 3D World

Welcome to this course on Symmetry and Structure in the Solid State. This would be a 12 week course which is offered under NPTEL which means that there is a total of 30 hours which we spend to cover the essentials of symmetry and structure determination.

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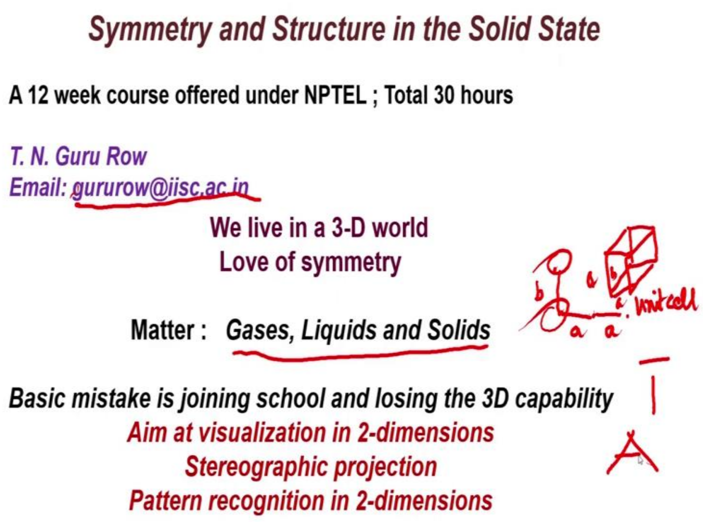

And of course, since we say it is solid state; it will be referring to solids and particularly crystalline solids. The questions if you have any during this entire course and so on can be addressed to me on the email, which the address of which is given here this is gururow@iisc.ac.in

Let's make a beginning; in fact, we have to always begin at the beginning so that we can reach an end. And this total of 30 hours now will be covered by understanding the 3 dimensional world in which we live in. There is one issue that is associated with the 3 dimensional world that is symmetry and both man and nature have a love for symmetry.

Symmetry is something which exists all around us and we grow as a part and parcel of symmetry. And therefore, getting a basic idea of what is symmetry is all about is essential. And of course, we have to formulate laws, rules and of course, the mathematics that is behind understanding symmetry. So, that any type of symmetry which occurs both in nature and in the man-made materials will be understandable in terms of these issue of symmetry.

Man always loved symmetry because whatever constructions we did and whatever constructions we continue to do; there is always a angle which is given to understand and appreciate symmetry in any construction we make. Nature also kept this in mind as we see from the way in which the trees grow, the plants grow and so on. But if we go to the very closer details of symmetry, we find there is a considerable amount of asymmetry.

In fact, it is the asymmetry which makes symmetry more appealing and this is of course, observed in many cases. Like for example, in particularly in south of India; they put a black dot on the face of the child during the birthdays or first year birthday celebration and so on. Now the fact, that there is a black dot introduces asymmetry, but this allows you to appreciate the symmetry.

So, the baby is supposed to be appearing more and more beautiful; of course they say it is the blessing of god and also the darting of the evil; which is why they put this black dot. But essentially the black dot is enhancing the symmetry that is associated with the baby’s face for example. And that's how symmetry is an issue which has to be understood both in terms of symmetry and the asymmetry which as a consequence appears.

In materials it so happens that the presence of asymmetry is the one which is required to give a property for a material. The most symmetric material is always not very interesting from its property point of view. So, if you want to imbibe a property to a material; it is essential that you introduce the asymmetry associated with a given material. So, material design, material construction also involves the loss of symmetry. What is more interesting is symmetry encompasses more or less all aspects of science.

Be it biology, be it material science, be it physics; in fact I teach a course where people come from all parts of the institute, all departments who attend this particular course because understanding symmetry is a fundamental issue which is required in order to pursue any kind of research in future. So, that way this is a very fundamental course and

I will keep in mind that the participants who are in this program also are coming from different disciplines.

There may be people coming from biology who probably had mathematics even at the 12 standard level and therefore it is essential that these people who are at the attending this course will also get a flavour of the entire understanding of symmetry. Now, symmetry also as I mentioned dictates the structure of the material and therefore, symmetry and structure go hand in hand. And the concept associated in this course will be to build the symmetry and structure in order to understand the solid state associated material.

Now what do we mean by a solid state? In fact, matter exists in 3 forms gases, liquids, and solids. These are the 3 forms of course, there is a fourth state of matter which is the plasma; which we will not touch in this particular course, but other than that there are 3 states are matter. In gases, it so happens that the particles which constitute the gas or not in contact with each other; they are very independent of each other.

And therefore, the particles are free to move for example, like air in this room. And the air in this room is spread the particles are all over this room; suppose we have opened the door, the air goes out of the room and then balances its pressure with the external world outside air and therefore, there is an issue of particles being completely free. So, if one wants to study the structure of this particle; then it is possible with gases we because we can study the structure of one isolated particle.

The methodology and the experimentation; however, becomes extremely difficult in order to study one single particle of a gas, particularly with the fact that a given temperature and pressure conditions let us say the normal temperature and pressure conditions; these gas particles are moving with enormous speeds. And therefore, arresting them in one place and studying the structure becomes an issue. It is not; I am not saying that it is not possible to study gas structures, in fact people have studied gas structures by variety of methodologies. By for example, creating a very high vacuum and in that particular work vacuum; this one single particle can be analyzed and there are methodologies that are developed.

When gasses now are taken and compressed; let us say we apply pressure on gases or we apply reduce the temperature. So, 2 parameters the thermodynamic parameters, temperature and pressure can now convert gases to liquids; in most of the cases not in all, but in most of the cases gases can be converted to liquids by application of pressure or reduction in temperature.

As we go to lower temperatures the particles now which are totally free to move around become somewhat connected to each other and that is how the particles in a liquid are connected to each other and liquids flow. So, when liquids flow the particles move along with it, and that is how they find their own level. For example, the water in this bottle finds it on level; that is because the particles inside the liquid are connected to each other.

However, even at in the normal temperature and pressure conditions; if we want to study a liquid, it is still difficult because we have the so called Brownian motion which we have studied in our high school days which keeps these particles not at rest, they will be moving at a certain kinetic energy. And this therefore, then again becomes a challenge to study these materials in the liquid form. Now we take the liquids and further compress it with application of pressure or we can also reduce the temperature and again as I mentioned most of the materials go from liquid to solid state.

Now, in the solid state the particles are in contact with each other and they are also so close to each other that they get arrested in their positions; respective positions. So, their movements are restricted; except for a certain amount of vibration which it can have about a mean position. So, all the particles therefore, find their mean positions and if these mean positions are found in such a way that one particle is connected to another particle at a distance a; let us say in 1 dimensions.

Then if this next particle also comes at a distance a from the second particle and so on in both directions, then we say there is a 1 dimensional lattice. A 1 dimensional lattice which is occupied by these particles and these; particles therefore, which occupy this 1 dimensional lattice or now arranged in such a way that there is a periodic repetition of these particles at a distance a; so, if we consider that in 1 dimensions then we see that the repetition of a units.

For example, if I say here there is a particle here, there is a particle here, there is a particle here; the distance between these two is 'a' and the distance between those two is 'a' then this periodicity we call it, this particular definition defines the periodicity. So, the periodicity is a; for this particular lattice of repetitions which are occurring terms of particles.

So, it is now essential therefore, to see whether we want to stay the idea is to study the structure of this particle. So, if you want to study the structure of the particle we know in a solid that this part in this particular type of solid; where there is 1 dimensional periodicity; we know that there is an order. Now because of this order the particles are arrested in their positions; they are not now moving around freely. And so it is possible now to focus on that point and determine the structure of that particular particle.

Now if this repeats now itself in 2 dimensions; lets say we go in this direction and this is b and the particle repeats again periodically in that direction. Then we have a 2 dimensional lattice where the particles are occupying the lattice points. And in third dimensions it so happens that since we live in a 3 dimensional world as I already mentioned; it so happens that in that particular direction also if there is a repeat pattern, then this forms now a unit which we always not write in 3 dimensions, but write in 2 dimensions, because we are used to 2 dimensions as I will mention in a minute. We are used to 2 dimensions and so we write the 3 dimensional object in this form.

So, we say that this now is a 3 dimensional crystal; this is a 3 dimensional crystal because this now repeats a along the one direction, b along the second direction and c along the third direction. So, the repetition a, b and c now will keep going through the 3 dimensional space and develop it into a object. Now this object if it happens like that with a, b, c as the periodicity repeat periodically repeating distances; we call this a crystalline solid. And so we now restrict our discussions for some time until we mentioned later that the discussions will now be centered on crystalline solids.

So, we consider in this particular course the symmetry and the structure associated with crystalline solids. See one of the restrictions that automatically come on to the nature of the particle; the particle is not necessarily let us say a dot, it could be an object, it could have some shape like that let us say. So, the dependence of the particle is now the same particle will repeat here again like that, but then the distance between these two is maintained.

So, the crystalline state therefore, will arrest these particles with the periodicity that is required to repeat in all 3 directions. And this now becomes an essential factor because this is the one which puts certain restrictions on the way in which the particles are arranged. So, the restrictions come from the nature of the; what we call as this box which eventually we will define later as the so called unit cell.

So this now is referred to as a unit cell and if this repeats in all 3 dimensions to form the full crystal. So, it is therefore, essential to study what is the content of this unit cell rather than study the entire content and that is what we will do when we go to the structural aspects of these materials. So, as I mentioned that when we are looking at 3 dimensional objects; we try to write the 3 dimensional objects in a 2 dimensional projection.

This is the mistake we made by joining school because when we went to school on the very first today itself; grim looking teacher took a stick in one hand and the chalk in the other hand and they started telling us what is a straight line, what is a bent line. So, they said right a straight line, horizontal line, a vertical line and then they took another vertical line and another vertical line; put them at an angle and put third vertical line and said this is alphabet a.

So, we learnt in this particular way whatever we have learnt in the school. And therefore, what happened is the 3 dimensional; we were born in a 3 dimensional world, but the 3 dimensional understanding which was there probably till we went to the school is lost completely. So, we now are comfortable with 2 dimensions. So, there are 2 ways in which we can visualize in 2 dimensions and see still try and understand the symmetry aspects.

One is of course, what is known as stereographic projection; we will see in a minute how it looks like. And the other one is the so called pattern recognition in 2 dimensions. So, we will spend some time on both these issues; stereographic projection we will do it in detail later on when we go and try to study the symmetry elements in more detail. What are the topic typical symmetry elements which occur in crystalline solids; when we look into that we will look at stereographic projection. The pattern recognition in 2 dimensions we will look at in the following slides.

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Rubens Aguilon: Stereographic Projection

So, this particular slide is an interesting painting which was drawn by Rubens Aguilon and this is a picture which I took from the library museum the Louvre Museum in Paris and this is hanging on the wall. And you see that it is not just us who are having problems in understanding the 3 dimensional structures even the Gods had problems.

So, here is the picture of Atlas who carries in Greek mythology the earth on his shoulder. And then they want to find out let us say the distance between Bangalore and Mumbai on the surface of the earth. So, what is happening is that this angel is shining some light and that light is creating a projection and the 2 angels are measuring now carefully with a divider the distance between Bangalore and Mumbai.

So, essentially what this is done is showing is that it is possible to steady 3 dimensions in 2 dimensions to start with. And then we have to therefore, find out the rules and regulations which govern the stereographic projection which we will study later on not right away; we will study later on probably in the coming classes. So, in this particular class we will also look at the visualization of symmetry in 2 dimensions.

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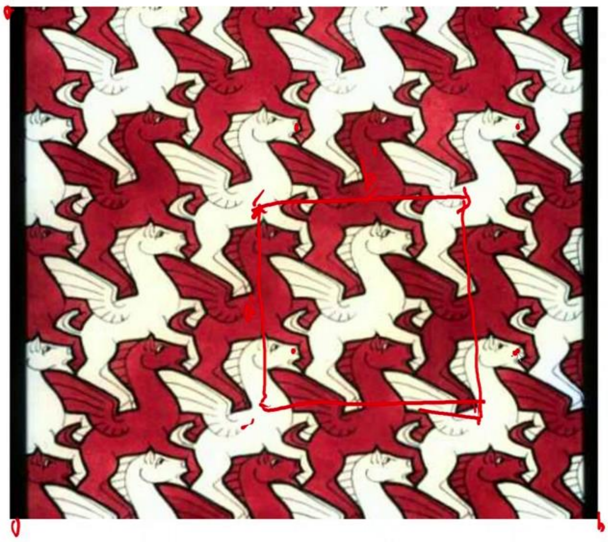

And that will come from the next slide which is showing us the actually it is a diagram which is drawn by a person called EC Escher; who of course, unfortunately passed away recently.

He made these abstract paintings of course, he is not a crystallographer, but he made these abstract painting with which we can understand all aspects of symmetry. In fact, more or less all the aspects that we need to describe the symmetry and structure in the solid state. And so I am going to show you several of these diagrams and then if people are interested in looking at the detail of this; this particular set of pictures there is an IUCr book which is issued which is available which gives you a list of all the EC Escher diagrams.

And all these diagrams are somewhat abstract and somewhat imaginative. For example, here you see the flying horses, you have a set of white flying horses and a set of red flying horses; the white ones here and the red ones there and these flying horses now, repeat themselves in this 2 dimensional motifs. So, if you now start this as a 0 of the of our mapping; then you call this as the a direction and this as the b direction for example.

Then in this a direction and b direction we have this motif and this particular motif has a repeat pattern. For example, we get this white horse; repeat itself at this position and repeat again here, repeat again here; this is at a certain fraction of a and this is at a certain fraction of b. Now this fraction of a and that fraction of b with respect to the a and b which we have marked here is essentially representing the unit which will now repeat itself in 3 dimensions; in 2 dimensions to describe the entire motif.

So, we take lets say the stomach of this horse; the stomach of the horse and probably I have drawn it a little closer it should be the stomach of the horse here and the stomach of the horse there. If we take that, that unit if we take; it will now we take this unit displace it to this position, displace it to that position and so on; we will generate the entire motif. One of the beauties that is associated with this is also the fact that there is no empty space in this.

So, it is completely closed packed; so when we are looking at crystalline materials also when materials crystallized like you know the flying horse can be replaced with a molecule, the molecules try to now arranged in such a way that they are close packed. This is the property of the fact that we need to have a solid when the particles have to be in contact with each other and if the particles have to be in such a way that they repeat in both a and b directions uniformly; then we will see that it has to have a close packing.

So, if we call this as a prime and this as b prime then we have this unit a prime b prime representing the repeat pattern. What is very interesting also is this is the fact that instead of taking the centre of this horse; as I have written we can take any part of the white horse. We can take the nose of this horse, the nose of that horse, the nose of that horse and the nose of that horse and define the so called unit which repeats itself and that unit will be identical to this unit.

So, we can take any part of the white horse; likewise we can take any part of the red flying horse. So, if we take any part of the red flying horse and then show from red flying horse to the next line red flying horse that repeat will also be the same and this is known as translational periodicity. So, the periodicity with which it repeats in a direction and b direction is now controlled by an operation a symmetry operation which is now referred to as translation operation.

So, this entire motif is now dependent upon the fact that we built these units and translate these units by a certain amount a prime along this direction and b prime along that direction. We can go either in the positive way or in the negative way; it remains one and the same. So, therefore we now therefore describe this 2 dimensional motif in this particular manner.

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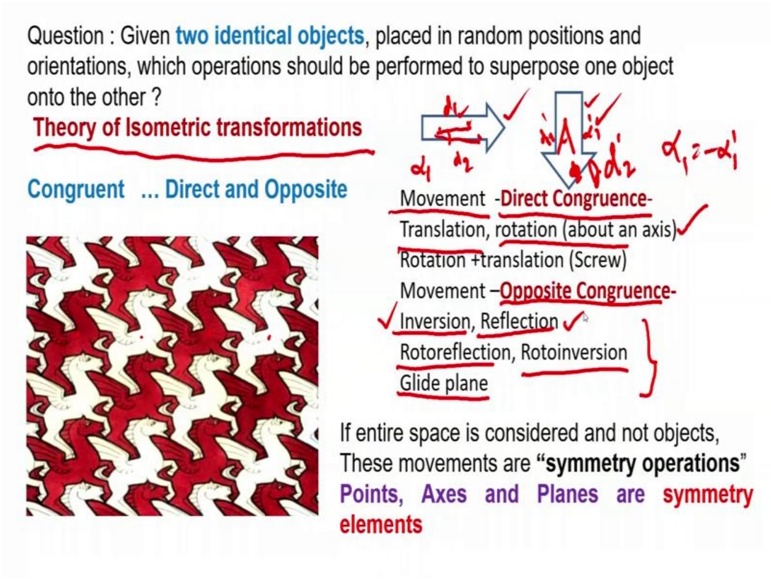

The next slide will tell you how to do; how to see that 2 objects are identical. We have been telling that this white horse is identical to this white horse and the red horse is identical to that red horse. When can we say that 2 objects are identical? This is an operation which this is a explanation which comes from serious mathematical considerations and that is the theory of isometric transformations.

So, we are not going into the detailed study of theory of isometric transformations because that is the one which tells you when you can, given 2 identical objects placed in random positions and orientation; which operation should be performed to superpose one object onto another. Now this is a very basic question, when we say 2 identical objects; how do we define this identity with respect to the 2 objects?

So, there are 2 types of identities we can define one and there referred to also as congruent objects. Now we say this is one object, this is another object; these 2 objects are what we call as congruent objects because in all principle definitions these 2 will be 2 identical objects. Now we have drawn 2 arrows one in this direction one in opposite direction; so the directions are different.

So, the way in which we have to prove that this is identical to that one is to use this concept of movement. So, we use this concept of movement; so by moving we have what we call as the; in case of direct congruence we move it using the translation which we described; we translate the object. We can also rotate the object about a certain defined axis; we can also do the rotation combined with translation. So, these operations which we do; the moments which we do the whatever movements which we do these are referred to as symmetry operations.

So, we have object 1, object 2; so what we do is we translate this object in the in the given direction and then rotate it about a position about an axis and then the rotation plus translation combined will orient this object along this direction. And these 2 then will be called identical objects; provided they are congruent with respect to each other. So, if we cannot have the shape of this object like the shape of the object is immaterial in this particular case because the way we define it is the following.

Suppose we take a point here on this object and another point there on the object and draw the distance the distance between these 2 is d 1; that is a vector which we draw. And we take another point here and draw and join these 2 points and call it as d 2 and the angle between these 2 we call it at alpha 1. And then a similar definition of identical identity will come if we take in this object on this particular object; similar positions occur in such a way that we have a d 1, we have a d 2 and an angle alpha 1. We call this as let us say alpha 1 prime this is d 1 prime and d 2 prime.

So, by definition the d 1 and d 2; so d 1 prime and d 2 prime. So, if d 1 is equal to d 1 prime and d 2 is equal to d 2 prime; alpha 1 is equal to alpha 1 prime, then we say that these objects are congruent and there of direct congruence. So, in all case cases of direct congruence the moments will be either translation or rotation about an axis or a combination and of rotation and translation; which is referred to as the screw.

So, these movements will now bring in the objects onto direct congruence. The opposite congruence the second type of congruence that can exist is the so called opposite congruence where again d 1 will be equal to d 1 prime d 2 will be equal to d 2 prime, but alpha 1 will be equal to minus of alpha 1 prime. Such objects are referred to as objects which are identical and they are of opposite congruence.

As we see here the moment for opposite congruence will be involving an inversion; inverted the object about itself there is a reflection across a plane. And then there is a rotation followed by reflection; a rotation followed by inversion and the so called glide plane where we not only have a translation, but we reflect it about a plane. Now the details of this we will work out as we go along in this particular series of lectures. So, if we are talking about independent objects here; 2 identical objects; so if the 2 objects are identical we call these moments as symmetry operations; if they operate on the entire space and then the symmetry elements therefore, will be either points or axis of rotation or planes of rotation.

So, the entire space therefore, now can be considered as a symmetric space with the following symmetry operations. The symmetry operations could be with respect to a point we have an inversion and with respect to axis we can have a rotation; we can have a reflection about a plane and the combinations of these. So, points axis and planes therefore, form the so called symmetry elements.

I think this brings us to more or less the end of the first half hour. And so I have in this half hour tried to cover the basics of what are 2 identical objects. And in what way these identical objects will be of congruence and how this congruence can be direct and opposite. And what are the symmetry operations which take an object from of direct congruence onto itself, opposite congruence onto itself.

So, in principle the entire space therefore, is consisting of these symmetry operations. So, a 3 dimensional space now is not just a 3 dimensional space; this 3 dimensional space let us say if there is inversion, it has a centre of inversion, a point at which the inversion takes place and so on.