Crystals, Symmetry and Tensors Professor Rajesh Prasad Department of Materials Science and Engineering Indian Institute of Technology, Delhi Frieze Group-II

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There was a famous mathematician John Horton Conway. So, he was also interested in many, many things in mathematics if you just google on Conway you will find 1000 of websites devoted to what Conway has done he was also interested in the symmetry and phrase groups and for phrase groups he developed these footprint motifs and also gave them some nice memorable name.

So, if you hop on one foot in this case the left foot. So, somebody is hopping on left foot with black paint on it. So, he leave footprints like this. So, what it is symmetry of this hop print what is translational symmetry very good. So, anything other than, so translational symmetry is represented by a lattice. So, if we select a lattice point and you know that lattice point is really your choice the pattern only dictates the translation that after what distance the lattice points will repeat but where you begin your lattice point what point you consider as your reference is of course your choice.

So, in this case let us say if we select maybe this gaps at the lattice point so all these points are translationally equivalent and distance from one to other is a lattice translation vector. So, there is a translational periodicity and the other symmetry it has does it have a mirror plane or 2-fold, 2-fold is there it has no symmetry other than translations. So, that is one kind of pattern and remember we are talking of frieze groups which are space groups of 2 dimensional patterns. So, footprints are 2 dimensional pattern but with only 1 dimensional periodicity.

So, frieze groups are 2D patterns with 1D periodicity and we had started looking at it and we had looked at some beautiful patterns border patterns in the last class and we saw 5 of them. But we had claimed that there are 7. So, these are examples of space groups you can call it a space groups, because they are combination of translation and point symmetry like rotation and reflection.

So, it is a special kind of space group when we talk of space group without any qualification we essentially mean 3 dimensional space group of crystals with periodicity in 3 dimensions. So, the object is also 3 dimensional, crystals is 3 dimensional and periodicity is also in 3 dimensions, because it repeats in all 3 directions. But in frieze group first of all the object is not 3 dimensional but only 2 dimensional and even 2 dimensional object can have 2 dimensional periodicities like in floor tiling's or wallpaper.

But in frieze group although the pattern is 2 dimensional but translation or periodicity is only in one dimension this is what you are seeing and this particular the hop pattern is having only translations and that is a minimum requirement anyway for any periodic pattern. Then the second one Conway has called spinning hop, what do you see here? What kind of symmetry? 2-fold and translation? So if we consider let us say let me identify the 2-fold.

So if we you will let us say join this thumb to this thumb and this heel do this heel the intersection point will define the 2-fold and same similar thing will happen in the next motif the 2-fold will repeat it will repeat with the because the pattern has translational periodicity the pattern repeats by this distance translational periodicity. So, 2-fold also will generate unless and until 2-fold also repeat by the same distance you will lose the translational periodicity. So, the 2-fold also is getting generated at this distance but is that all.

Student: Inversion Sir, around 2-fold if we keep Z as 0 then x y z goes to minus x minus 5.

Professor: And what does 2-fold do? Same. So, in 2D that is an interesting point you have raised. So, let us make a note of that in 2D the 2-fold and the inversion are the same they are not distinct operations whether you say invert in a point so just like you were saying that I have suppose I say that this is 1 bar point this is an inversion center.

So, what will it do to any vector? Any vector r it will rotate sorry it will invert to minus r. But now I say I do not think of inversion operation but I think of 2-fold rotation operation. So, it will rotate this vector by 180 degree and will again give you the same minus r. So, whether 2fold or whether inversion center acting in 2D have exactly the same effect same mapping point to point mapping is exactly the same the matrix if you write.

So, the matrix you write by looking at what it is doing to 1, 0 and 0 1, 1 0 it will invert into bar 1 0 and 0 1 it will convert into 0 bar 1 the 2-fold rotation also will take 1 0 to minus 1 0 and 0 1 to 0 minus 1. So, their matrix also is exactly the same, mapping is exactly the same, only our thinking is different, in one case we are saying that we are inverting and in another case we are saying that we are rotating by 180 degree. So, crystallographers have decided to exclude 1 bar from the notation in 2D and in 2D we only use the 2-fold.

So, if you have 2-fold? Yes, you have inversion center trivially there. So, we will not count it has another symmetry operation. What is that all here all we or missing some symmetry in the spinning hop, spinning hop see I think Conway is imagining a still hopping because nobody will have his 2 feet like this unless and until at some devil or that 1 foot backward and 1 foot forward. So, he is imagining that you are still on 1 foot, but you are spinning and jumping on the other side and then again you jump so you are doing a hop and spin so spinning hop. So, is that all the symmetry in the spinning hop?

Student: 2-fold in the middle 2-fold in between.

Professor: 2-fold in the middle what we are missing is that will be join this thumb to this thumb or this big toe I think and this heel to this heel. You will find that there is a 2-fold there also let me use a different color to show that 2-fold. So, you have a green 2-fold there. And last class we had tried to prove this also I think since myself forgetting that whether I had proved it or not I can excuse you for forgetting what was the content of that whenever you have a combination of a translation and 2-fold rotation you will generate 2-fold not at the translation distance but at T by 2.

So, let me say that 2-fold at origin combined with a translation T is a 2-fold act T by 2 away from the origin. So, this probably is a nice operator symbolism we can see. So, this will always generate so in any pattern where you have 2-fold and translations very, very important result and you will see the repetition of this, in any pattern where you have 2-fold and a translation combined with that you will find that actually 2-folds are appearing at half the translations. And those two 2-folds I have given different color here from pattern wise also if you see they are differently located with respect to the pattern.

So, here you can see that the red one is between two vertically shifted footprints. They have footprint just above and below the red one has footprints above and below the green one does not have footprints above and below it shifted the left and right. So, in the pattern they are also playing different roles both are 2-fold. See if you try to take a mirror image now these footprints are difficult to draw.

So, let us suppose I put you want to put a horizontal mirror or vertical mirror, you want to put a vertical mirror. So, let me put a vertical mirror here then if I can draw my drawing skills are being challenged. Somebody good in drawing should do this maybe something like this you will get is not it you can see that none of the footprints are in this orientation none of the footprints. Here you have 2 variants but you do not have this variant.

That the curvature, the curved side or the deeply curved side is upwards and the toes are on the right. So, whenever the deeply curved side is upward like in the lower row the toes are on the left. So, you do not have a mirror image you have only rotated version than the mirror image this. So in this case you do not have left handed and right handed or left foot and right foot both are actually left foot only. That is why it is still a hop you are hopping is still on one foot only you are spinning. So it is rotating by 180 degree. Yeah hop is or 2-fold will be a type I operation. So, it cannot change the handedness of the motif. Student: Rotation translation, I mean do these operations have something fundamental property that they cover anything else? Or is there anything else possible that we define a new operation and then include that into (())(14:26). So, for example, inversion is something I defined a new operation which is does not exist. And then take that symmetry corresponding to that operation also into the symmetry group.

Professor: So, I think the current list of symmetric operations is complete. That is one that we made for crystallography, for crystallography we said that we are limited to 1, 2, 3, 4 and 6 because translation was not allowing 5 and translation was not allowing higher than this also, and then 1 bar, 2 bar, 3 bar, 4 bar, and 6 bar. So, for and we said that of course there is translation so this list is more or less complete except for the fact that we have not considered a screw and glide which I have been mentioning here and there but I have been avoiding discussing this screw and glide.

So, now after years of work can thinking and all this list is supposed to be complete that is you cannot think of a new symmetric operation which cannot be described by these it will be if it is and I think there are just like we gave a mathematical proof that for lattice translations for periodicity no rotations other than these are allowed. So, similarly you can give proof that no other symmetric operation can be present other than these.

There can be composite operations. So, for example you can combine a screw rotation to a glide reflection and will get something new but that is still the components are known you can that we anyway know that if we screw is the symmetry of the crystal and glide is also a symmetry of the crystal then the space group is just again the symmetry group and by the closure property of the group any combination of the operations have to be some operation.

So, it may appear new at the first sight some combination may and translations are infinite rotations are finite. So, you have only a finite number of rotations but translations are infinite and they are at various angles in 3D. So, I can have a rotation about this axis and can think about translation at some angle and what will that give. So, it may give something which may appear to be new at the first sight, but then it has to be a combination of my list of group elements which I have listed.

If it is satisfying the group property and since it is symmetry it has to satisfy the group property because by very definition of symmetry we are demanding that the object is left invariant comes into self-coincidence, one operation brings it into self-coincidence, another operation brings it into self-coincidence. So, the combination has to bring it into selfcoincidence one followed by another.

So, we do have means I think your worry was probably here that 2 bar became, sorry 2 became 1 bar is that how do we know whether we are having a new one or an old one in the new garb?

Student: Why we are only taking this subject for example go to inversion rotation. So, why not own other possible oppressions we are taking all possible operations.

Professor: We are restricted to rotation and rotor inversions only because translation restricted to these and it is a good question I think we have not answered this.

Student: maybe that comes out to these combinations of.

Professor: So, rotor reflection when we considered we showed that rotor if each rotor reflection is corresponding to some rotor inversion. So, we found nothing new. So, we gave up or we accepted. So, and 2 schools of initially developers came so (())(20:14) for example he is a famous crystallographer and one notation is (())(20:19) notation. So, he took rotor reflection, he did not consider rotor inversion. But later on when these international tables people came they considered rotor inversion. But in the end just like in the 2D case, 2-fold is becoming 1 bar, in 3D you know that 1, 1 bar is 2-fold rotor inversion. In 3D 1 bar is not 2 in 2D 1 bar is 2, but in 3D 1 bar is 2-fold rotor reflection that turns out to be the same means.

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Spinning Hop FI 2,T = 27/2 $\begin{pmatrix} \overline{1} & 0 \\ 0 & T \end{pmatrix}$ $\begin{pmatrix} \overline{1} & 0 \\ 0 & 7 \end{pmatrix}$ 12346 12346 T Jump T+ m₁₁ Screw Glide (F) 10 Sidle Ö 1=2 $T + m_L$ 0 * Spinning Jump I=2 $T + m_1$ ~) (~ ~) (~ ~) (~ ~) (~ ~) (~ ~) (~ 0 Spinning Jump $T + m_L + m_{ll} + 2$ 0 0 () NPTEL



If you suppose you have an object here at r inversion will take you to an object there of a chain handedness if you do a 2-fold rotor reflection so you will first rotate by 180 degree to bring it here handedness will not change and then you will reflect and you will find that you will reach exactly the same place again with the turn the reflection the rotation did not change the handedness but the reflection will change. So, what you are showing that 1 bar is 2-fold rotor reflection.

So, our naming will change depending upon our preference or something. But in terms of mapping, we are not getting any new mapping the same point is being mapped to the same point in exactly the same fashion. So, yes the all these worries were there but your question is still a little deeper which we have not answered and probably assuming it to be true or taking

it for granted or brushing it under the carpet whatever you call it is that what we are requiring demanding it symmetry, symmetry does not change distances that is one big restriction.

Because otherwise if you think mathematically of mappings, mappings can distort your object also means if you deform a ball into a cube that is also mapping each point of the ball to some point of the cube but there the distances will change. So, the first thing requirement of symmetry is that it is an isometry, isometry means distances are not changing.

And the second requirement is that it is an isometry which maps the object to itself. So, an isometry which maps object to itself is a symmetry operation you can then show what you are demanding and we have not done is that now if we say that this is the only requirement what all possible mappings are there in 3 dimensional space or in general in n dimensional space which will satisfy these two criterion that it does not change the distances and it maps the object to itself.

So, and I think that sort of mathematical questions are also answered you we have not taken that route and sort of have just assumed that these are the operations for each operation I know that it is not changing the distance and it is mapping the object to itself. So, that we are verifying but we have not given a proof that these are the only operations and we have exhausted the less this is what you are demanding.

So, we can look that look it up. I hope that there are theorems and things to prove that in more mathematical texts we should be able to find it. So, now let us come to jump. So, here both foot are there. So, you can see now the left foot and the right foot both are there. So, obviously there is a reflection horizontal mirror in jump we have horizontal, horizontal mirror and of course the translation anyways there.

But now the 2-fold rotations are not there because the upper foot and the lower foot cannot be related by rotation because there is a change in handedness and rotation will not change the handedness as soon as you will rotate you can see compare it with the spin as soon as you will rotate the foot will start pointing on the other side instead of forward direction it will start pointing in the backward direction the only way to keep both foot pointing in the same direction is to reflect in a horizontal mirror.

So, but then if you reflect the left foot change into a right foot so that is the jump. So, this is translation plus I can see a mirror which is parallel so a parallel mirror then of course he has to generate a vertical mirror also. So, for that you will have to do a sidle you have a mirror

translationally equivalent mirrors are here but again identical theorem and these you these you can prove by Seitz notation which we have developed.

So, mirror also gets generated. So, actual lattice translation is T but mirrors will be repeating by T by 2 this will always happen there is no violation and you can see it by using the matrix and Seitz notation then of course there is this interesting spinning jump. So, you are having both foot on the floor but you spin and jump so the next time you are pointing after jumping when you put your foot down you are pointing in the other direction.

So, what do you have here? So, you have both vertical and horizontal mirrors. Anything else? Some more mirrors T by 2 mirrors and where, now this is again something you can prove whenever 2 mirrors are intersecting at 90 degree to each other the line of intersection of the 2 mirror has to be a 2-fold. So, I leave this as a homework again for using Seitz notation or you can use a simple geometry also I think we had done this in some of the earlier class.

So, if you have let us say we have 2 mirrors and let us play with the motif here. So, the mirror, the vertical mirror will generate another motif of a different handedness. Then both of these will reflect in the horizontal mirror and handedness will once again change. But now you can relate the object of same handedness by 180-degree rotation about the center so you can see that is a 2-fold and that is you are spinning jump so here we have. So here we have translation plus perpendicular mirror.

Now we have translation plus perpendicular mirror plus parallel mirror and the resulting 2folds this seems to be the most symmetric and we seem to have exhausted our ingredients. Because in 1D translation because we have to preserve the line, I have no other rotation than to fold. Because I want to bring the line into self-coincidence whatever I do, I want to bring line into self-coincidence that is the definition of symmetry. And if I have a line and if I give any other symmetry operation, 30 degree is 60 degree 90 degree I get a totally different line it cannot come into self-coincidence.

So, the only symmetry operation which was available to us in terms of rotation was a 2-fold rotation and mirror was available, but again mirror was available only in two specific orientations, either a perpendicular mirror which will reflect the line into itself or a mirror, which is passing through the line which we call the parallel mirror which will preserve the line any other mirror at an angle or something will till the reflected image into some other line.

So, we these were the things we had translations anyway were required because we were thinking of periodic patterns, then we used 2-fold to create a spinning hop then we created jump using parallel mirror, sidle using perpendicular mirror and then we combined everything to get a spinning jump. So 5 different frieze groups. So, what else can be there now, are we missing something?

Think of all the things you can do with T you can hop, you can spin hop mostly will not try. But you can try spin hop will be a good exercise, jump, sidle or spinning jump. I think it will be a good exercise to go back to your rooms and try all these motions. Good symmetry homework. Are we missing something? Normal walk, we are missing the normal walk. So that is where comes this step in a normal footprint you will not do any of those (())(32:52) you will normally walk like this.

So if we are doing normal walk like this does it have a 2-fold anyway 2-fold will relate only right foot to right foot and left foot to left foot. The left foot chain is on the top. So somehow one foot has to be rotated one left foot has to be rotated to another left foot by a 2-fold. But 2-fold will change the direction of in the direction in which the foot is pointing here all the feet are pointing to the right.

If I apply it 2-fold the foot should be pointing to the left no foot is pointing to the left here. So 2-fold is out. Perpendicular mirror can we consider? A perpendicular mirror will relay a left foot to a right foot. And again will change the direction in which the foot is pointing here left foot and right foot both are pointing in the same direction. So there is no perpendicular mirror.

Parallel mirror will change left foot to right foot and it will be pointing in the same direction. So here do we have left foot and right foot and both are pointing in the same direction. So there was a possibility of a parallel mirror. But what happened? The parallel reflection would have come vertically below the foot. So, it is not coming vertically below the foot. So, what is happening? It is reflected very good. It is reflected as well as translated. So, the most important way of walking actually and we cannot say that this pattern is not symmetric so it does not have parallel mirror also since it has none of the ingredients which with we started we clear that this is a non-symmetric pattern but it does have translation, translation is there.

So, then we say that a step is having the same symmetry as the hop. But, that looks a little far-fetched because internally we do feel that this pattern is showing something more

symmetry than a hop even without the lower row it was a hop with the left foot or even without the upper row it was without the upper row it was a hop with the right foot.

So, it does have a symmetry and this is the kind of exploration and something which your question was pointing to that how do we know that we have exhausted means we could have been satisfied with this that we have explored everything and we have all the symmetry and announced to the world that there are only 5 possible frieze groups but when you look at it you will find that actually you have discovered now a new symmetry where you are combining a translation with a reflection.

So, you have the so called glide plane or in 2D a glide line and what you are seeing that you will, see you have to translate this by this much to get translationally equivalent foot or translationally equivalent motif so that translation is this but if you translate just half of that and then reflect you will get this foot then translate half and reflect you will get that foot, translate half and reflect so half translation is going this way neither the translation now the translation associated the translation associated with the glide operation is half the lattice translation.

So, if you do a half translation, the pattern will not come into self-coincidence, you have to do a full translation to bring into self-coincidence. So, half translation is not a symmetry operation. If you reflect in the red line again you do not get self-coincidence because without shifting it is not coming into self-coincidence. So, reflection is also not a symmetric operation of this pattern.

So, neither the mirror alone nor the half translation are symmetry operation but a combination of the two is a symmetry operation and that is what is called the glide operations. So, glide is a combination of half translation plus a reflection in a line containing the translation. So, this step gave you that example glide so this is the sixth one.

Finally, now can we combine now have, we have found a new thing glide. But we have three old things 2-fold, perpendicular mirror and parallel mirror. Can we combine our newly found glide line with one of these old ones to generate a new symmetry? Can I combine glide line with a mirror parallel to the line? What will happen if I combine glide line with a mirror parallel to the line? We can do means drawing these feet are difficult.

So you can take a simpler exercise. So suppose this is a glide line and you have an object. So, you reflect and translate you create an object since you reflected you will create an object of

opposite handedness then you again reflect and translate. So, you will get the object of same handedness then reflect and translate opposite handedness, reflect and translate same handedness. So, you are seeing the actual translation actual periodicity of the pattern is this whereas for glide what we were doing, we were giving only half translation.

So, if we just translate halfway then I will have to have a motive there which is not there. So, half a translation is not consistent but now if I want to make this line glide line into a mirror line let us say I make it a mirror line so which means the mirror will now create a new motif because it has to reflect this has to reflect here and this has to reflect here it has to reflect here so you get a plane mirror so glide means mirror dominates.

So, glide plus mirror is actually just mirror so it does not give you anything new what about glide plus 2-fold or perpendicular mirror can we combine glide with a perpendicular mirror try it in this way only the way I have shown you create a glide first create some motif which represents the glides and you add a perpendicular mirror what will happen so these new motifs you will generate trying to satisfy the glide.

So, you will find that again just like it happened with the combination of, see you have put a mirror plane with a glide is there or not this mirror plane is seeing a translation and the translation was of T so currently the mirror plane which I have drawn is with translation T because this motif is equivalent to this motif. So, that is your lattice translation. So, the mirrors are also separated by the same distance T but you know a combination of a mirror with a translation generate mirror at T by 2 which I have not yet drown they come there my placing is not perfect but you can imagine that there are mirrors there.

But there is something more can you see something more which is relating these motifs, between 2 mirrors now 2-folds are getting generated when I say 2-fold it is not only for the nearby motif any motif in that in finite pattern if rotated by that 2-fold any given 2-fold will give you equivalent motif somewhere else in the pattern. So, between 2 so red mirrors were generated by lattice translation the green mirrors got generated by that combination rule that a mirror with translation will always produce your mirror at half translation.

And then this blue 2-folds are also getting generating by some combination rule means I cannot avoid that I did not try to create 2-fold I just added one this red mirror plane but effect of adding the red this is where the space group is coming in, the effect of adding one single read mirror generated and infinitely many read mirrors at spaced by translation T because I

have to preserve translational periodicity then a translation in combination with a mirror gives you mirrors at T by 2.

So, I get infinitely many green mirror planes. And now all these conspire to give you 2-folds exactly in between the 2 neighboring mirrors between a red mirror and a green mirror. So, you generate a totally new kind of symmetry by combining this newly found glide line with one of the older symmetries and that is a perpendicular mirror and that is Conway spinning sidle.

So, if you look at this pattern now you see these are the vertical mirrors, this is the horizontal glides and then these are the 2-folds between the mirror plane in fact in my previous to use the color coding of my previous drawing I can use green, so a spinning sidle. So, 7 different symmetry and there are no more now one can claim that there are no more again without proof we are saying just by our intuition we have tried to combine but by intuition we were ending at 5 then glide was discovered.

We can of course, we can say that we combine glide with we cannot glide with parallel mirror that was a trivial case that became mirror we combined glide with a perpendicular mirror. And we got this interesting situation of spinning sidle. What about if we combine glide with 2-fold that is our another masala but then you can see that combining it with a mirror generated automatically 2-fold. The reverse will also be true. If you started with a glide line and combined it with a 2-fold. That will generate these mirrors.

Even more interestingly, if you did not have the glide line and you just have combine a mirror with a 2-fold not passing through the mirror that will generate the glide. So, if I have a mirror I started with a mirror you can do these experiments, because we see that is why it is important to do the 2D space groups a little bit more carefully because nothing is beyond your imagination. Nothing is outside your plane of paper there is nothing which you cannot draw and see in 3D you have to imagine a lot but the 2D cases can be fully worked out with just with the pen and paper.

So, in 2D cases you can so what I was saying the experiment let us try to do that. I claimed that suppose you did not have the glide you just had a mirror and a 2-fold. Only requirement is that a 2-fold is somewhere sifted from the mirror it is not on the same line then you can draw a perpendicular line from the mirror to 2-fold and show that this line is going to become

a glide. Why? Let us, let us try that I start with a motif here, a reflected motif here, a 2-folded motif here, another 2-folded motif there.

Now, a rotated mirror because if it is a 2-fold it will act on the mirror also where will it take the mirror by rotation about 2-fold, 2-fold is there a mirror is there if you rotate it the mirror will go on the other side at the same distance. So, that is exactly where these 2 motifs are anywhere demanding that they are connected by a mirror reflection once this is also a mirror this will reflect it will act not only on this lower motif it will act on this upper motif also.

So, this will reflect here with changed handedness this will reflect further apart again with changed handedness. And there will be a mirror again there. You can see now that your real translation from motif to motif is here. But you can also see now that you can take this motif by T by 2 and reflect in this plane to get this motif. And same thing is true for all. So, we did not start with the glide plane. We only started with the 2-fold and the mirror but we are seeing that glide plane is emerging spinning sidle.