Crystals, Symmetry and Tensors Professor Rajesh Prasad Department of Materials Science and Engineering Indian Institute of Technology, Delhi Lecture - 28 c

Physical properties represented by second rank tensors are Centrosymmetric

A very interesting result of the symmetry of physical property is that if any physical property is

represented by second rank tensors, they are centrosymmetric.

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Whether the crystal is centrosymmetric or not, we have seen that out of 32-point groups of a crystal, only 11 are centrosymmetric, 11 centrosymmetric point groups and the remaining 21 are non-centrosymmetric. They lack Centr of symmetry. But if a physical property is represented by a second rank tensor, for example, electrical conductivity, it does not matter whether the crystal has the centre of symmetry or no, the property will always have the centre of symmetry. So, second rank tensor property always has a centre of inversion, whether the crystal adjust to that centre or not. So, this is an additional symmetry you can see.

If the crystal has centre of inversion, then property should also have centre of inversion that is assured by Neumann's Principle. But if crystal is not having centre of symmetry, then this still property is having a centre of inversion. So, that falls into that category, that property must include the crystal symmetry, but may have more symmetry. So, for 21 non-centrosymmetric crystals, the property, second rank tensor property having a centre of inversion is an additional symmetry.

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So, why is this the case? Let us have a look. Look at it. So, first, as we said that property having a centre of inversion means if we have the axes, so let us say that the property was measured in some axis system x1, x2 and x3. And let us introduce another axis system which is related to the first axis by inversion. So, I invert all axes in the centre. So, the red and the blue axes are related to each other by a centre of inversion in the origin.

The property having centre of inversion means that if I represent the property in any of these two axis system, the property will remain the same. It will not change. That means the tensor, the second rank tensor, will remain the same during this coordinate transformation. So, let us see what is the A matrix for this transformation. The coordinate transformation matrix, so we write x1, x2, x3 on top.

The old on the top, x1 and x2 prime, x1 prime, x2 prime, x3 prime on the right, and we simply note all the direction cosines for these pair of directions, the cosines of angle between these pair of directions. So, x1 prime, if we choose x1 prime, x1 prime makes 180-degree with x1, cos 180-degree is minus 1. So, I write minus 1 there. x1 prime is perpendicular to x2 cos 90, 0. x1 prime perpendicular to x3, cos 90, 0. So, that gives me the first row.

Now, focusing on x2 prime, similarly, we see that it is 0, minus 1, 0 and x3 prime gives 0, 0, minus 1. So, this is the A matrix relating these two coordinate axes. And if we say that the property is centrosymmetric, then the property should not change under this coordinate transformation. So, let us think of a general tensor T which is represented by its nine components. So, if we now transform this tensor by the coordinate transformation, I should get the same tensor.

So, how is that true? So, we have seen that the coordinate transformation, the transformed tensor T prime, it is written as A, T, A inverse. We have also noted that A in the orthogonal transformations, A is always, A inverse is nothing but A transpose. So, we can write A transpose but not the particular values of A. In this case, A is nothing but negative of an identity matrix. So, if you note that, so all you have to do is instead of A, you have to write minus I, T and minus I transpose, which is minus I, T and another minus I.

So, you can see that this becomes plus I, T, I or plus T, because identity matrix does not change the matrix to which it is being multiplied. So, T prime turns out to be exactly the same as T under this coordinate transformation. And what was the coordinate transformation? Coordinate transformation was relating a centre of inversion. So, that means the property has the centre of inversion and we did not worry in this derivation whether the crystal wall having the centre of inversion or not. So, any second rank tensor property will always be centrosymmetric. Thank you.