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Lecture - 7 Physical Properties of Crystals (Continued)

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Last time we wrote the transformation rule for vectors in the following form, if A i prime are the components of A vector A in an primed coordinate system, and A j are the corresponding components of the same vector in an un-primed coordinate system, then if these two coordinate systems are related by A transformation coefficient A i j, then the transformation rule for the components of A vector quantity A connecting the components in the two coordinate systems is given by A relation of this form A i prime equal to A i j A j, where the reputation over the subscript j implies summation.

And A i j's are the direction cosines of the coordinate axis in the primed system with respect to the corresponding axis in un primed system. So this is the general transformation rule and this immediately enables as to generalized the definition to tensor quantities of higher rank.

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For example left T i j be the components of A second-rank tensor, we saw last time that electrical conductivity electric permittivity electric susceptibility these are all quantities which correspond to second rank tensors. So let T i j represent any tensor T of second rank, where the subscript psi j run over one, two, and three; in three dimensional space as we already seen such A second rank tensor is something that connects to vector quantities A i and b j A i and b j are the components of the vector quantities, A and b in A given coordinate systems, and this T i j gives you the connection between these two for example j equal to sigma e where which defines the electrical conductivity may be returned index form by sigma i j e j, where e is the electric field so sigma i j is the tensor quantity which relates j i to e j.

So this is A general form of such A tensor. And now we want to find how the tensor transformation how the tensor quantity T i j transforms under A coordinate transformation A linear coordinate transformation so for this we start with the definition of T k l prime the same tensor quantity specified not in the un-primed coordinate system but in the prime coordinate system such A tensor quantity is obviously would be relating A similar would be following A similar relation in the primed coordinate systems may be A k prime equal T k l prime b l prime where k l run over again one two three so that would be the relation between the A k prime and b l prime why are the tensor quantity T k l prime in the primed coordinate system now we know

that there is the transformation rule for A vector quantity so i know how A k prime and A i are related A k prime all that we do is change this dummy indexes.

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So I can write A k prime equal to A k and i need on this side A i A k i A i that would be the similarly I have b l prime is A l j b j so these would be the transformation rule for the vector A and b in terms of the coefficient A k i and A l j i again i j k l running over one two three as before so suppose I start from this and write A i as T i j b j. Now from this I can write the inverse transformation as A a l j b l prime, so that I can replace this sphere and write A k i A l j T i j b l prime and this is what we say is given by these, so this is equal to T k l prime b l prime, so from this I can see at this quantity corresponds to this.

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$$T_{k\ell} = a_k a_{\ell} T_{\ell}$$

So I can write the transformation rule T k l prime equal to A k i A l j T i j that would be the transformation rule for A tensor quantity A prime two so now we know looking at this and this we can generalize this transformation rule for A tensor of any arbitrary higher rank so suppose i have T p q r r s etcetera[noise] can be written as A p i A q (j A r k A s l etcetera[noise] T i j k l etcetera where the subscript's correspond to A tensor of any arbitrary high rank so that is the general transformation rule for A tensor quantity T of arbitrary rank so that will give the general rule using this transformation equation table gives you A few examples giving the rank as A tensor and then they corresponding transformation rule forward or backward that is the new component when you make A transformation from A prime unprimed to A prime coordinate system what will be components of this tensor in the primed coordinate systems in terms of the old prime unprimed component in terms of the new components.

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So the this is just A straight forward application of this rule in next table list's some important physical properties examples of various physical quantities and they are rank or order and the corresponding defining equation for example pyroelectricity pyroelectricity is establishment (refer time: 11:00) of an electric polarization when you increase the temperature of a sample, so the pyroelectric coefficients that corresponds to tensor of rank one or a vector whereas as we already seen quantities such as the electricity conductivity electric susceptibility magnetic susceptibility thermal conductivity these are all tensor's second-rank for the corresponding transformation rule is given in the last defining a equation is given in the last column then for as examples of tensors of rank three you have a direct piezoelectric coefficient we all have heard of the how piezoelectricity generated, and an electric field is establish when certain crystals are such as quartz are subjected to pressure, so that is the piezoelectric.

And you can have an indirect or reverse piezoelectric phenomenon in which A instead of A pressure generating an electric field an electric field sets of A pressure so this is use for A example in the application of piezoelectric quartz crystal it is used in stabilization of high frequency an electronics circuits so in this you have the these are all examples of tensors of rank three then as I discuss last time elastic modulate such as the elastic stiffness or the elastic compliance which defines the relation between the elastic stress and strain or vice versa there

corresponds to tensors of rank four, the next come to an important concepts of how the symmetry of A crystal affects physical properties of the crystals.



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Now, we have seen that are tensor tensor of rank zero namely A scalar has just one component which is the magnitude of the scalar quantity whereas the tensor of rank one which we is more commonly known as A vector as three components three independent components this you will remained ourselves this is nothing but the four one then the tensor of rank two as in general three square equal to nine common independent components, and so on so in general the tensor of rank n as three to the power n independent components.

Now if you have a such a large number of independent component it should be rather difficult that is where the symmetry of A crystal enables as to deal with A much smaller number of components independent components so a tensor so that the life becomes simple this influence of symmetry on the number of independent components that are physical property mean process is governed by what is known as neumann's principles according to which the physical property of any crystal must include the symmetry elements of the point group of the crystal it can have symmetry which is more than that but it must at least have the symmetry of the point so to know whether a physical property process a certain symmetry or not we must determination the physical properties for example electrical conductivity relative to some fixed axis in the crystal then the symmetry operation has to be performed on the crystal for example A rotation about given axis then the physical properties should be again determined making the measurement in the same direction as before if the symmetrical properties remains the same after the symmetry operation has been performed then that physical properties is process that particular symmetric neumann's principal says that the symmetry elements of A physical property include those of the point for the crystal. We have already discuss the various point groups to which various crystals along this means that the physical property may process more symmetry then the point group in fact many cases it is in did...

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Ao now we can see how this symmetry influences the number of independent component that have given physical property in A process for example let us consider as few simple example start with we all know that there are so called doubly refracting on birefringent solids crystals in which the refracting index has not just one value but two values. (Refer Slide Time: 17:25)



And if it is usually because of the fact that such A crystal such A by birefringent crystal as A unique A point corresponds to A point group which has A unique axis of symmetric which involves A rotation about A particular axis so this rotation may be A twofold rotation A threefold rotation and A fourfold rotation or six fold rotation so in that case when you have such A unique axis it made

sense to see is A matter of common sense to see that there is refractive index will have A particular value if it is measured along that particular axis of symmetry and if you go in the plain perpendicular to the axis of symmetry then the value of the refractive index slightly to be having A different value so this is all birefringent arises. So this is one simple situation where one can readily intuitively understand that the number of components such as the two component of A refractive index will depend on whether that solid process axis of symmetry or not similarly if you have A complete the cubic symmetry for a solid such as sodium chloride for example is an alkali alight which possesses a cubic symmetry, so if you have A cubic symmetry than you can see from again intuitively understand from the on the behavior of A cube that it has A symmetric behavior in all three orthogonal crystallographic axis x y z or A b c.

So, you have the same behavior because this is cube possess symmetry in all these three orthogonal directions so one can intuitively expect that the physical property which should

possess the symmetry elements of this cubic solid should also have the same value A along the three directions so all the three independent which are normally independent components of this physical property will now have A single value so that there is only one independent value for the physical property in this case so these are all matters where we can intuitively understand that they higher symmetry of A crystal will correspond to A reduction of the number of independent components that that physical property may have.

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Next coming to the electrical conductivity sigma i j which we will write have to in full as sigma one one sigma one two sigma one three sigma two one sigma two two sigma two three sigma three one sigma three two and sigma three three, so this is the array of nine independent components for A tensor A second-ranked such as the electrical conductivity but we can show that the electrical conductivity tensor is not just any second rank tensor that it is a symmetric second-rank tensor in other words sigma i j equal to sigma j i if you apply the electric field in the direction j and measure the current density along the i th direction you get sigma i j but if instead you apply the electric field along the i th direction. And measure the current density along the jth direction you get sigma j i and intuivation again tells us that these two will be the same because of the symmetry with respect to the 1 reversal of interchange of cause and effect so because of this, we can readily see that the components sigma one two and sigma two one and sigma one three and sigma three one and sigma two three, and sigma three two they are all identical so that

these nine independent components really reduced to a set of six and the others are just the same so they are no longer independent. So we have only six instead of nine we have only six independent components in this case, so now this number still is high but depending on the additional symmetry of the physical property which includes the symmetry of the point group of the crystal the number of independent component may get further reduced for example in the case of A cubic solid which we saw we have all the components are the same and we have just one number so the number of independent components are the electrical conductivity reduces to just one in this case, so that is why a cubic solid is an isotropic solid it doesn't exhibit an isotropic it has the same value in all the three directions.

If you have a crystal of for a cubic solid so the number of components is just one in this case if you have a crystal of uniaxial symmetry and if the three the axis, which is symmetric is taken to be the third axis then we will we can readily see that the number of independent components will be just these one component one value along the three axes along the axis of rotation along the axis of uniaxial symmetry and another one in the the plane perpendicular to this is the case with conductivity or refractive index and so on such an axis is known as the optic axis that the high symmetry present reduces the number of independent components we can see this in A bit more quantitative way by the following discussion of this effect of symmetry.

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Suppose IO have A four fold axis or A two fold axis let me take A two fold axis suppose this axis is A two fold axis this is along the z direction which we take as the third direction this is A two fold axis along z or three directions if the crystal possesses such A twofold axis then we can readily see that the presence of the two fold axis along the z direction means that we have A transformation before adopt the rotation which are given by so become minus x one this becomes minus x two while x three remains the same, so that is the transformation rule which we can readily see from the general rule of cos theta general transformation metrics of cos theta sin theta zero minus sin theta cos theta zero zero zero one where theta equal to pi this is substitute the pi you get this result so these are the transformation rules which governed a components are the coordinates in the case of a twofold axis along the z direction.

So this means that the transformation this twofold rotation changes one to minus one two to minus two and leas three the same suppose we consider the electrical conductivity this means sigma one one will transform, now to sigma minus one this will become minus sigma one in this case but there will be also be the other one and that will again become minus, so this will again go to sigma one one the two negatives two minus one the product of two minus one plus one similarly for sigma two two remains the same sigma three three of course remains the same but if we come to things like sigma one two again that will be the same because go to one and to become minus one and minus two therefore the product will again remain the same but when we go to sigma one three only one goes to minus one and three remains as plus three so this will be minus sigma one three and the only way if the physical property have the symmetry; these two should be equal so the only way A quantity sigma one three can be the negative of itself used by its vanishing identically leaving behind only the other four components these are the only nonzero components for A two fold axis which can do the same thing for any combination of symmetry elements which we have discuss in the case of point groups.

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We will take up two specific situations one is the electric coefficients and the other one is the elastic model and examine in brief the (refer time: 30:00) consequence of symmetry on this the governing equation for the p so electric coefficients for where i j k run over one two three d i j k's are the p so electric coefficients p i is the polarization components and sigma j k are the components are the applied stress tensor, so the general equations governing the are known now if we want to go further we introduced for compactness the matrix notation simplifies this free subscripts notation into A two subscripts notation for which will simply write one one becomes just one two two is two three three is three.

And then two three and three two are replaced by four with that we can write this tensor in A much more compact form so that and then we can examine how this various components under symmetry there are now because it is a tensor of third-ranked with symmetry connections there are eighteen p so electric coefficients in general, but depending on the symmetry is the crystal the number of independent coefficient get reduced as we have discussed in the case of A simple example like A twofold symmetry for example for uniaxial symmetry it can be shown that there are only three this reduces to three for uniaxial symmetry and this is what makes life somewhat easy for example p so electric trans gives us made of the ceramic p z p have such A symmetry that they possess one unique axis and there are three d coefficient the p so electric coefficient

which are corresponds to the so-called longitudinal more the transfer more and the share more similarly when we come to elastic constants this is A forth rank tensor.



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And we have A rotation like T i j equal to c i j k l sigma k l s k l these are the stress and strain relay coefficients and there can also be A reverse relation connecting the strains to this stresses so defining the elastic compliance now here again we can in general have thirty-six e because this is A tensor of forth rank we can have thirty-six independent coefficients which reduced to in the case of A case of A cubic solid so there will be only three for a cubic solid, so you can see that the symmetry can cause a considerably a drastic rotation of the number of independent component which one has to specify in order to specify the components of a physical property this is the main results of such analysis for a tensor physical properties corresponding to different tensor are summarized in the next table that we will just mention that ah the number of independent completely described a given physical property.

So one can in general the to specify the principal components in what is known as the principal coordinate axis system which whose in A principal coordinate systems for example for a tensor of rank two you how to specify the three component principal components in such a coordinate system. And the orientation of this coordinate system with respect to the any other arbitrary

coordinate system, so this is how a second rank tensor is specified, so this is we have now seen the effect of crystal symmetry on the physical properties in this lecture.