Crystals, Symmetry and Tensors Professor Rajesh Prasad Department of Materials Science and Engineering Indian Institute of Technology, Delhi Lecture 83 Representation of Physical Properties of Crystals by Tensors

So, we will now discuss representation of physical properties in crystals by tensors.

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Representation of Physical Properties of Crystals by Tensors Reference: J. F. Nye "Physical Properties of Crystals: There Representation by Tensors and Matrices" Oxford Univ. Press

This is an important and interesting topic. And the reference which I am using for these lectures is a very famous book by Professor Nye J. F. Nye; titled also Physical Properties of Crystals: Their Representation by Tensors and Matrices. So, I will follow his presentation rather closely. (Refer Slide Time: 00:35)

Ohm's law and electrical conductivity Ohm's law V= IR DI nce Potential difference Resistance Of Resistivity (Material Proper

Let us begin with a simple physical property with which we are all familiar with; and that is electrical conductivity. And electrical conductivity has a connection with Ohm's law from which it is defined. So, and we have we are familiar with Ohm's law that V is equal to IR, where V is the potential drop or potential difference between two ends of a conductor, R is the resistance of the conductor, and I is the current passing through it. So, essentially it is saying that V and I are proportional, the proportionality constant R is the resistance, resistance of the conductor. The unit of resistance is ohm that of current is amperes and the potential difference is volts.

So, we can we have the relation that ohm is equal to volt by ampere. Now, let us try to look at this law in a little microscopic way and that is let us represent the resistance in terms of resistivity. Because, we know that the resistance is proportional to the length of the conductor L, and it is inversely proportional to the area cross-sectional area when this is area, and this will be the length of the conductor.

So, resistance is directly proportional to the length and inversely proportional to the area; and this proportionality constant is known as the resistivity. This is resistivity, and this is a material property. So, resistance you can see, since resistivity is a material property, resistance will depend upon the length as well as the area of the conductor; but the resistivity depends only on the material.

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Now, let us look at this resistivity little bit more microscopically. So, we will let us look at or formulate Ohm's law microscopically. So, V is equal to IR, let us divide both sides by length. And also let us divide the right-hand side by area; so, I multiply by A in the denominator and numerator. The idea is that V by L voltage drop per unit length is now can be identified by the electric field; it is the voltage gradient, and we can call that an electric field. And I by A can be written as j which is the current density. And you can see RA by L we had defined, R is equal to rho L by A, so rho is exactly RA by L.

So, we can write this quantity as the resistivity; so, we get the equation E is equal to j rho. Or, if we want to write it in terms of j, so current density is 1 by rho times the electric field, and we define the reciprocal of resistivity as conductivity.

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ΞσE 1 N vector electric fied (vector) $\dot{j} = \sigma E$ $\int_{Scalar} \Rightarrow \dot{j} \parallel E$ This is true in isotropic roraterial But not true in general.

So, in this microscopic formulation, we can see that we now have, we can write the current density j as conductivity times the electric field. Written in this way, we have written all quantities as a scalars; so, because they are only the magnitudes, but one should note that both j and E are actually vectors. So, it is a current density vector and it is an electric field vector.

So, if we put the vector sign on them, I am using underscore for vector sign; so, j is equal to sigma E. If we keep sigma is still a scalar, then it immediately implies that the current density vector j is parallel to the electric field vector E. This is the case is true in isotropic materials, but not true in general. Let us see why that is the case.

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0 Electrical conductivity high conductivity $\underline{J} = \underline{J}_{11} + \underline{J}_{12}$ Current density j A electric field E

So, we take an example of electrical conductivity of graphite. Graphite is highly an isotropic material and is made up of graphene sheets, which I represent here as these horizontal lines. So, let us say these are grapheme sheets. Now, in graphite we know that the electrical conductivity normal to the heat, this electrical conductivity is extremely high; whereas electrical conductivity parallel to the heat is low.

This is a high conductivity direction and this is a low conductivity direction. In this case, it will not be true in general that the electric field and the current density vector will be parallel. Let us look at that. So, let us assume that we are applying an electric field exactly at 45 degree to the normal direction. So, this electric field let us say this is E 45 degree.

Now, what will be the resulting J in this case? So, let us decompose this E into two components. E parallel, parallel to the basal plane, parallel to the graphite sheet; and E perpendicular, normal to the graphene sheets. Now, since I am taking the angle to be 45 degree, you can see that these two components will be equal in magnitude.

But, since the conductivity is low in the basal plane, the same magnitude electric field the magnitudes are equal; so, these magnitudes are equal. But, since the conductivity is low, it will give a small current in the direction of basal plane; the same field will generate a small current, so let me represent that by j parallel.

But, since the conductivity is high in the normal direction, the same magnitude electric field will be capable of generating a larger electric current. Now, you can see, since j parallel is much smaller than the perpendicular, they are not equal; the net resultant current density j, which will be sum of, vector sum of j parallel and j perpendicular.

This will not be parallel, it will not be 45 degree; because the two components are now no more equal. We are saying that j perpendicular is much much larger than j parallel. So, you can see that the current density is no more parallel to the electric field; current density j not parallel to electric field E. So, this is the general case in an isotropic material; the electric field and the current density will not be parallel. How do we handle this situation? So, let us try to if it is not parallel; so, in an isotropic situation, we could have written first write for isotropic situation.

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Current density j K electric field E For isotropic materials $\underline{j} = \sigma \underline{E} \quad \dot{j}_1 = \sigma E_1$ $\dot{j}_2 = \sigma E_2$ $J_n = \sigma E_3$

J was parallel to E, and sigma was a scalar electrical conductivity. If we write this in terms of components, then we will find the component j1 sigma times E1, j2 sigma times E2, j3 sigma times E3. So, these two sets of equations are equivalent; the here we have written in the vector form; and here we have written in terms of the components.

You can see that the j1 component the first component of the electric current density depends only on the first component of the electric field. Similarly, the second component of the current density depends upon the second component of the electric field, and the third one of j depends upon the third one of E. And in each case, the proportionality constant is the same; and is a scalar value sigma. But, in an isotropic case, we have seen that now; since, j will not be proportional to E, this relationship will not be true.

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So, for anisotropic materials j is not parallel to E. So, the components will now depend not on the corresponding component, but will depend upon other components also. So, j1 for example, will become a function not only of E1, but also of E2 and E3. What kind of function this is? Of course, the simplest function simplest function to assume is the linear case, which is the case in most of the time for small fields and small current densities.

So, we have the linear relation. So, j is linearly dependent upon E1, E2 and E3. Now, linear dependence means that it is proportional to all these components separately with some proportionality constant. So, let us write those proportionality constant in a systematic way, giving the subscript sigma11, sigma12, sigma13.

So, sigmall is the constant which relates E1 to j1; similarly, sigmal2 is the constant which relates E2 to j1 and so on. So, with this kind of convention, we can write the second component 21 E1, plus sigma22 E2. So, in the linear approximation the three components of current density, each depend upon the three components of the electric field; and we have these coefficients which you can see, because the j has the dimension of current density, and E has dimension of electric field. So, sigma all these sigmas, the nine sigmas I have written sigma11 to sigma33; all will have the dimensions of electrical conductivity.

So, they are some sort of electrical conductivity; but, to describe the property of the material, all these nine components will be required. To express the relationship between j and E, now, one scalar sigma one scalar conductivity is not sufficient; we require nine such coefficients. Now, let us interpret. So, these nine coefficients, we can write as a matrix; and we can call them nine components of the conductivity tensor. So, we are bringing the tensor here to describe that conductivity is not described by one in just one term or one scalar; but you require nine quantities to describe it.

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of Conductivity $j_1 = \sigma_{11} E_1 + \sigma_{12} E_2 + \sigma_{13} E_3$ $j_2 = \sigma_{21}E_1 + \sigma_{22}E_2 + \sigma_{23}E_3$ $J_3 = \sigma_{31} E_1 + \sigma_{32} E_2 + \sigma_{33} E_3$ $\begin{array}{c} J_1 \\ J_2 \\ J_3 \end{array} \stackrel{=}{=} \left(\begin{array}{c} \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{array} \right) \left(\begin{array}{c} E_1 \\ E_2 \\ E_3 \end{array} \right)$

Now, how do we interpret these terms? Let us say. So, let us write this equation; let us write these three equations in the matrix form. So, we can write it as, you can describe the current density vector as a column vector; and then we can have the conductivity tensor matrix; and then we can have the three components of the electric field vector.

The linear equation as we well know can always be written as a single matrix equation. So, in this matrix equation, this represents the current density vector, and this represents the electric field vector. And the physical property which is connecting the current density vector to electric field vector now is described by this nine-component matrix; and that will be called the electrical conductivity tensor. Now, let us look at the physical interpretation of these quantities. So, suppose we apply only electric field in the, so let us case take as a special case.

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Electric field is applied in the z-direction. $E_1 = E_3 = 0$ $E_1 \neq 0$ $\begin{pmatrix} J_{1} \\ J_{2} \\ J_{3} \end{pmatrix} \stackrel{=}{=} \begin{pmatrix} \overline{\sigma_{11}} & \overline{\sigma_{12}} & \overline{\sigma_{13}} \\ \overline{\sigma_{21}} & \overline{\sigma_{22}} & \overline{\sigma_{23}} \\ \overline{\sigma_{21}} & \overline{\sigma_{23}} & \overline{\sigma_{23}} \end{pmatrix} \begin{pmatrix} E_{1} \\ 0 \\ 0 \end{pmatrix} \stackrel{=}{=} \begin{pmatrix} \overline{\sigma_{11}} & E_{1} \\ \overline{\sigma_{21}} & E_{1} \\ \overline{\sigma_{21}} & E_{1} \end{pmatrix}$ $J_1 = \overline{O_1} E_1 \qquad J_2 = \overline{O_2} E_1 \qquad J_3 = \overline{O_3}$

Let electric field is applied in the x-direction; so, that means its component E2 and E3 will be 0. E1 will have a non-zero value. In this case, we can see from the matrix equation which we have. So, since E2 and E3 are 0, we can change it to 0. And then, you can see that you will get sigma11 E1, sigma21 E1, and sigma31 E1.

So, this tells us that if we apply an electric field E1 in the direction in the x-direction, then the current density in the same direction j1 is the current density in the direction of the applied field; and that is equal to sigma11 E1. So, this gives us an interpretation that sigma11 is nothing but the

electrical conductivity in the direction, in the x1 direction if the electric field is applied also in that direction.

Similarly, j2 is sigma21 E1. So, this tells us that sigma21 is the electrical conductivity which is connecting the electric field in the direction x-direction to the current density in y-direction; electric field in direction 1 to current density in direction 2. And finally, the third relation relates the electric field in the direction 1 to the current density in direction 3.

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| Tensor | Rank | No. of Components | Example |
|--------------------|------|----------------------|----------------------------|
| Scalar | 0 9 | aver 30 = 1 | density |
| Vector | 1 | 3'= 3 | polarization |
| 2nd rank tensor | 2 | $3^2 = 9$ | electrical conductivity |
| 3rd rank | 3 | 3 ³ =27 | Piczoelectric |
| NPTEL fensor | 4 | 3 ⁴ = 81 | Stiffner |

So, we have already introduced electric conductivity as a tensor; but they are in fact, the scalars and vectors can also be considered as tensors and tensors of different rank. So, in this table, I will simply write this term that a scalar is considered to be a tensor of rank 0. Vector is considered to be a tensor of rank 1; electrical conductivity, which we introduced as tensor is actually a tensor of rank 2. And we also can have tensor of third, fourth or higher ranks. The number of components for any tensor is scalar; you know that has just one component. So, the number of components is given as 3 to the power of rank of the tensor. So, 3 to the power 0 is 1; 3 comes from the dimension of the space.

So, since we are talking of three-dimensional space; so, a scalar will have one component 3 to the power 0 is equal to 1. We know that in three dimensions, vectors have three components. So, you can see that they can be treated as tensors of rank 1; electrical conductivity we saw was having 9 components.

So, 3 squared as 9, third rank tensor will have 27 components; and fourth rank tensor will have 81 components. A scalar you know many examples; so, let us say density. I will just give one example each vector; you have many vectors. Let me give one example, polarization vector; we already saw electrical conductivity as a second rank tensor.

Third rank tensor comes when we discuss piezo-electric coefficients; and fourth rank tensors comes in elasticity as a stiffness tensor. So, we stop here for this video, we will take up the discussion of tensors. We will continue the discussion of tensors in succeeding videos which will come after this. Thank you very much.