Smart Structures
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Week - 02
Lecture No - 07
3D Constitutive Modeling of Piezoelectric Materials -1

Welcome to the first lecture on constitutive modeling of piezoelectric materials.

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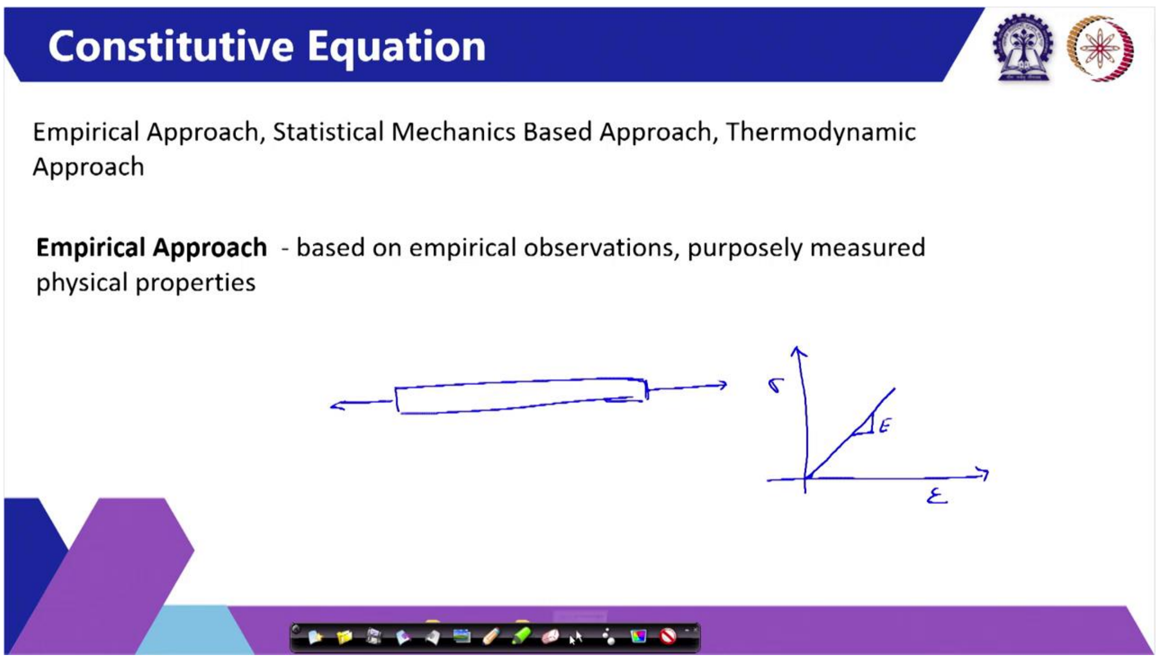

So, at first we will look at various approaches used for constitutive modeling. The first one is empirical approach, then there is statistical mechanics based approach and then there is thermodynamics approach. Now, empirical approach as the name suggests, it is based on some experimental observations. So, for example, if we think of a slender bar like this, steel bar maybe and then if I want to measure the elastic modulus we may put it on universal testing machine and measure its response and based on that we can draw a stress-strain curve like this. So, in this axis, it is strain and in this axis, it is stress and then if we are within the elastic limit, we may get a variation in this form.

Now, we can easily fit a straight line to this variation and we can say that the slope of this straight line is our Young's modulus (E). Now, this is quite useful for simple cases, but for relatively complex cases, where there are multiple variables or multiple dimensions, this approach is not that easy or that useful. So, in that case, we need other approaches.

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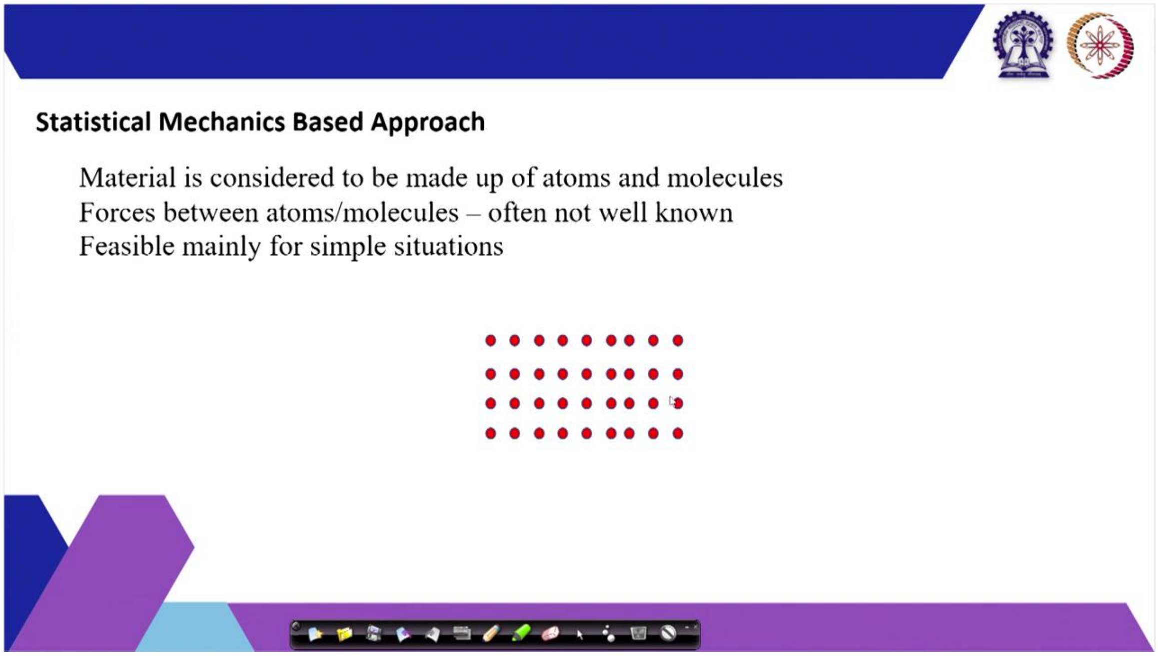

Now, among other approaches, there are statistical mechanics based approaches. Now, in the statistical mechanics based approach, the material is assumed or considered to be made of a lot of atoms and molecules and there are forces between these atoms and molecules and accordingly it is simulated, but again if the simulation takes a lot of time, so, they are feasible for simple cases only and also the forces between these atoms and molecules, they are often not well known.

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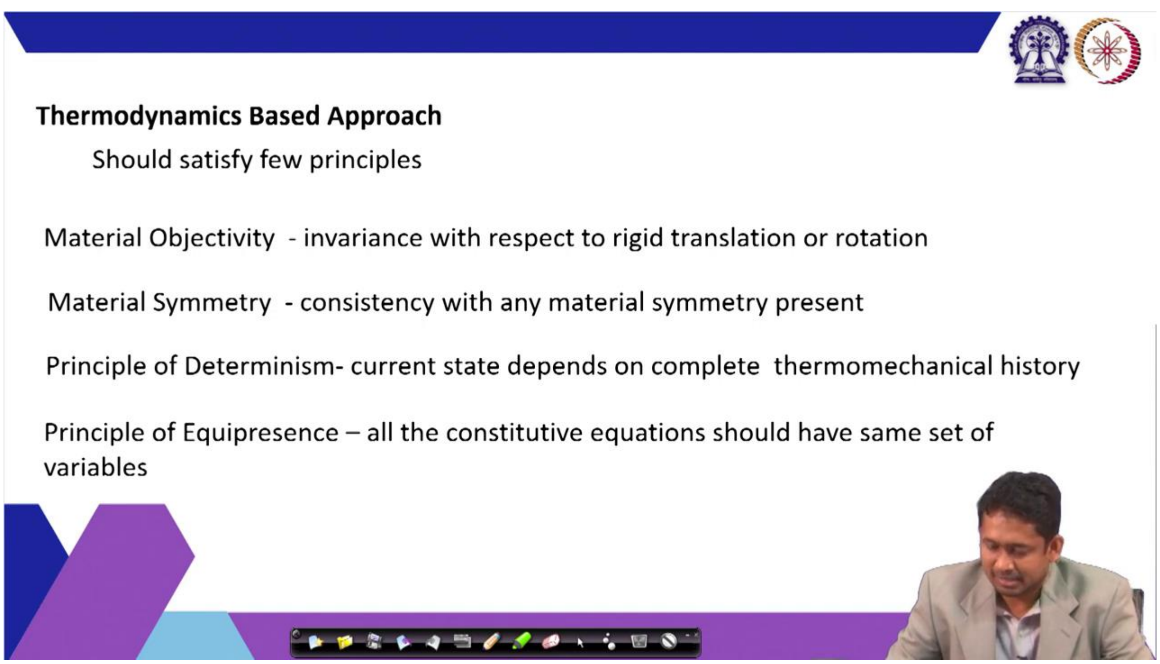

Now, there is one more approach that is thermodynamics based approach. Now, thermodynamics based approach requires that our constitutive model satisfying few principles. So, here are those principles. First of all, it should satisfy material objectivity that means, the constitutive relation should be invariant with respect to rigid translation or rotation.

In material symmetry, so, if there is any material symmetry, our constitutive model should be consistent with that. Now, comes principle of determinism. It says that the current state depends on the complete thermo-mechanical history. So, for example, if we think about the relation between stress and strain it says that stress at the present time should depend on the strain at all the previous time steps or in other words stress at the present time is not influenced by strain at any future time step. Now, we do not always need the entire strain history to compute the stress at the present time step.

For most of the cases or most of the simpler cases, our stress is dependent on strain only at the present time step. So, in our modeling also we will not consider the history dependence. So, we will assume that the quantities at the present time step are dependent on the other quantities at the present time step only.

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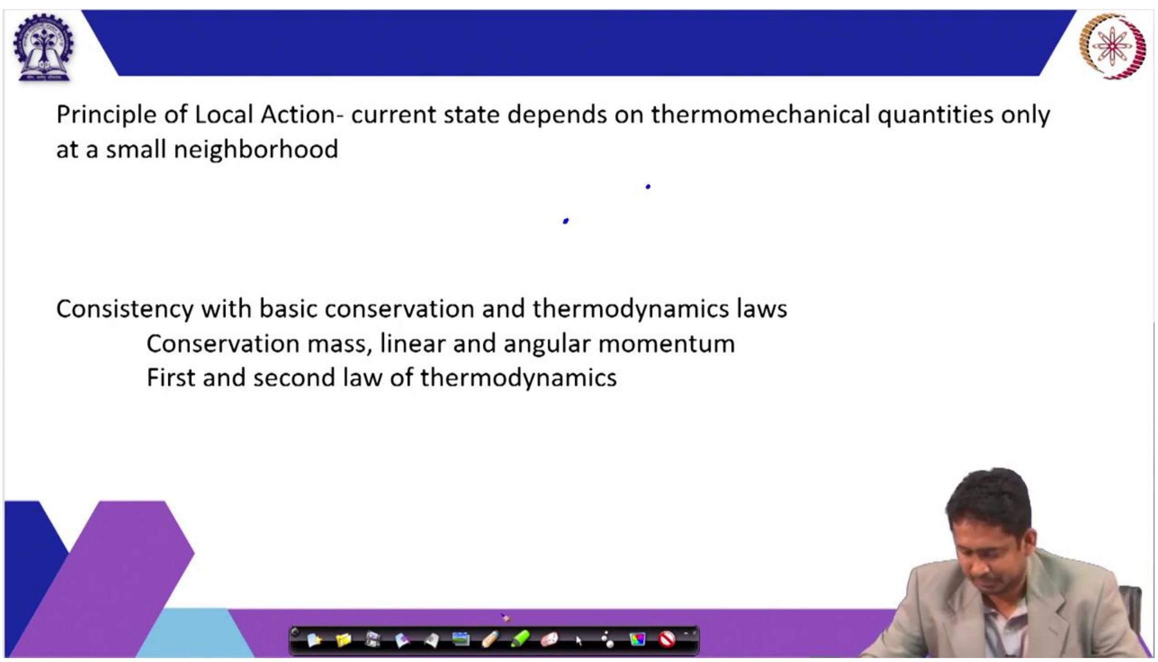

Then comes principle of equipresence. So, all the constitutive equations should have same set of variables. So, we will look into that when we do the constitutive modeling actually. So, we will see that these constitutive equations have the same set of variables. Then comes principle of local action. It says that current state depends on thermo-mechanical quantities only at a small neighborhood. So, again if you look at the stress strain example, so, if I want to find out the stress here, so, the stress here is not influenced by the strain here.

So, to find out the stress here we need strain also here only. Now, there is another subject called non local elasticity where we assume that the stress here is also influenced by strain at a far point, but here we are confined to local elasticity only. So, our stress here is not going to be influenced by strain at any other point. So, stress here will be influenced by only by strain only at this point. So, that is our principle of local action.

Now, our constitutive relation has to be consistent with some basic conservation and thermodynamics laws. So, these laws are conservation of mass, linear and angular momentum and there are first and second law of thermodynamics.

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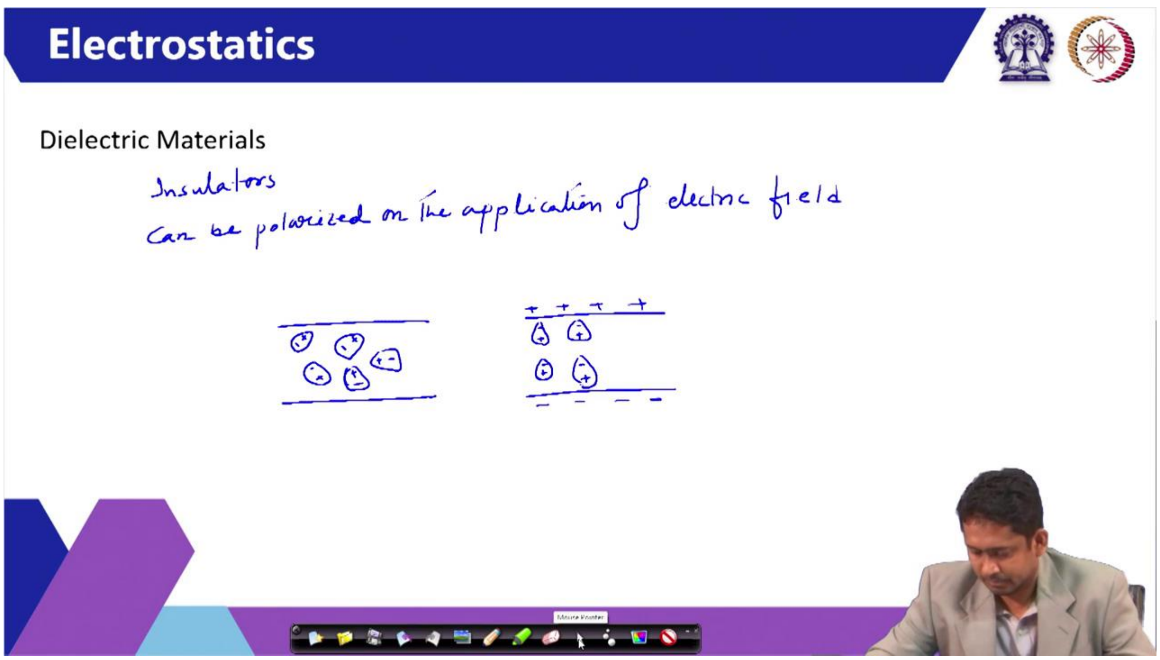

Now, we will start with the constitutive modeling. So, first of all, while dealing with piezoelectric material, there are mechanical quantities as well as electrical quantities. So, we need to spend some time on electrostatics.

So, to define various variables related to the electrical problem and their relations and then we will go to the conservation laws and all these findings from the electrostatics will be helpful there and then we will be in a position to derive the constitutive relation. So, our piezoelectric materials are dielectric materials. So, what is a dielectric material? So, these dielectric materials are insulators. So, they do not conduct an electricity because they do not have free charge and these materials can be polarized on the application of electric field. So, what it means is our dielectric materials have lot of these molecular dipoles.

This means that the center of the positive and negative charges is not coinciding. So, this is called a dipole. But these dipoles have a diverse orientation. So, they are randomly oriented and due to this random orientation, everything cancels each other. So, there is no net polarization.

Now, if we apply an electric field here, so suppose this side is positive. So, this attracts the negative charges and this negative side attracts the positive charges. So, because of that the orientation takes place in this form. So, all the negative goes towards this upper side and the positive comes towards the lower side. So, that way we can say that it gets polarized. Now, it may not be fully polarized. So, the polarized takes to a certain extent. So, to which extent it gets polarized ? It depends on the amount of electric field that we are applying and also the property of the material.

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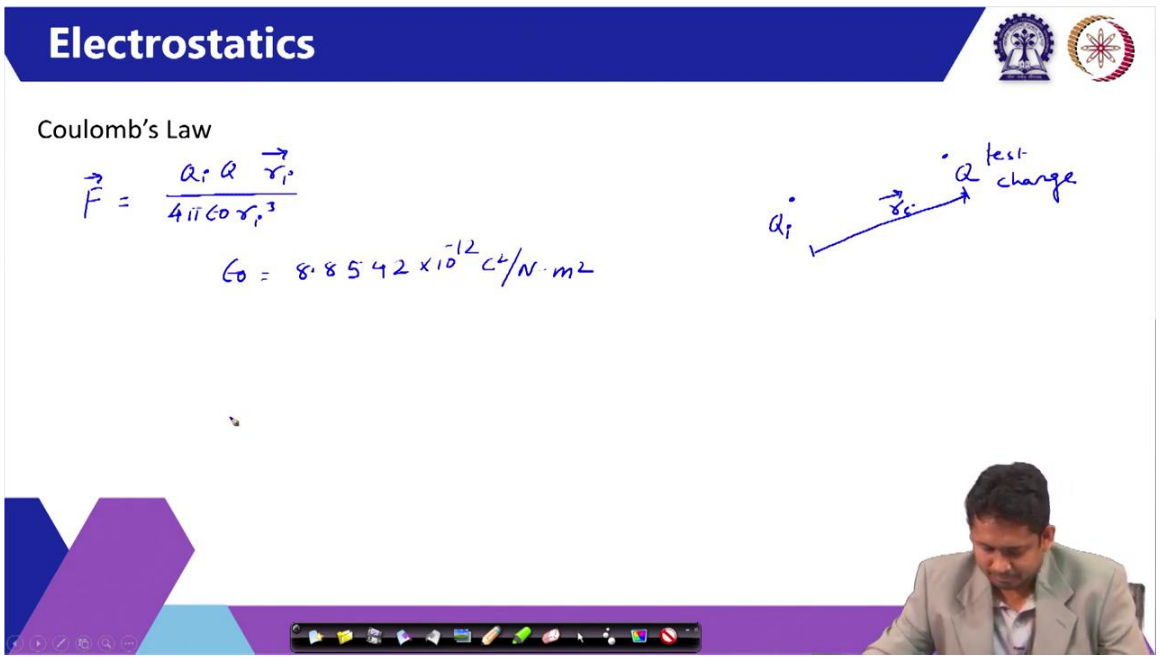

Now, let us come to Coulomb's law.

Now, Coulomb's law says that if we have a charge here Q, we call it Qi and if there is another charge Q, So, Coulomb's law helps us find out the amount of force this experience due to this or this experience due to this. So, the distance between these two are suppose r. So, we define a vector r. Now, the amount of force Q is experiencing due to Q_i can be written as – Qi Q by four pi epsilon zero ri cube multiplied by ri as a vector.

$$\vec{F} = \frac{Q_i Q \, \vec{r_i}}{4 \, \pi \, \epsilon_0 r_i^3}$$

So, this is r_i, the distance between Q_i to Q.

Now, we are finding out force here on Q. So, we call it a test charge and this is the expression for the force. Now, here epsilon zero is a constant and its value is 8.8542×10^{-12} $C^2/N\text{-}m^2$. So, coulomb is a unit of charge.

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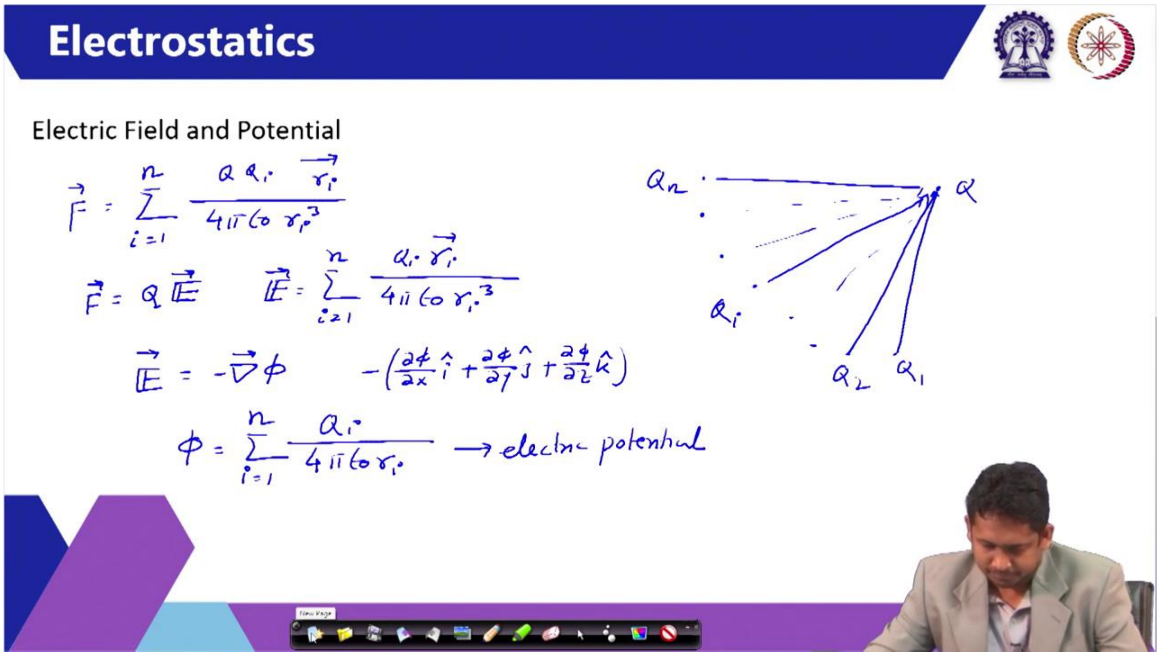

Now, we will define some quantities called electric field and electric potential. So, to do that let us assume that there are multiple of this Q_i's. So, I call it Q_1, Q_2 this may be Q_i and this may be called Q_n. So, there are n number of these charges and there is a test charge Q. So, you want to find out the force experienced by this due to these charges. So, those are that total force is nothing but a vector addition of all these individual forces.

So, we just have to write the previous expression, but with a summation sign. So, we know the force at Q the test charge due to a charge Q_i. So, now if I want to find the total charge due to i varying from 1 to n the total force is just the summation of it.

$$\vec{F} = \sum_{i=1}^{n} \frac{Q_i Q \, \vec{r_i}}{4\,\pi\,\epsilon_0 r_i^3}$$

So, this is our total force experienced by this test charge Q. Now, we define a quantity called electric field and by definition electric field is the force experienced by a unit charge. So, these are electric field. So, we are denoting electric field by this double struck E.

$$\vec{F} = Q\vec{\mathbb{E}}$$

Now, if I compare this expression with this expression, becomes the electric field vector becomes just this. So, this is the force experienced by a unit charge. So, I just replace Q with 1. So, the expression reduces to this.

$$\vec{\mathbb{E}} = \frac{Q_i \, \vec{r_i}}{4 \, \pi \, \epsilon_0 r_i^3}$$

Now, let us define something called electric potential. So, this electric field is a vector. It has 3 components. Now, this can be represented by gradient of a scalar and let us call that scalar as phi.

$$\vec{\mathbb{E}} = -\vec{\nabla}\phi$$

So, if I expand this quantity, it just looks like this –

$$\left(\frac{\partial \phi}{\partial x}\hat{\imath} + \frac{\partial \phi}{\partial y}\hat{\jmath} + \frac{\partial \phi}{\partial z}\hat{k}\right)$$

So, this is a vector and if I equate that with this vector, we can get an expression of phi and that phi comes to be this. This is our electric potential phi.

$$\phi = \frac{Q_i}{4 \, \pi \, \epsilon_0 r_i}$$

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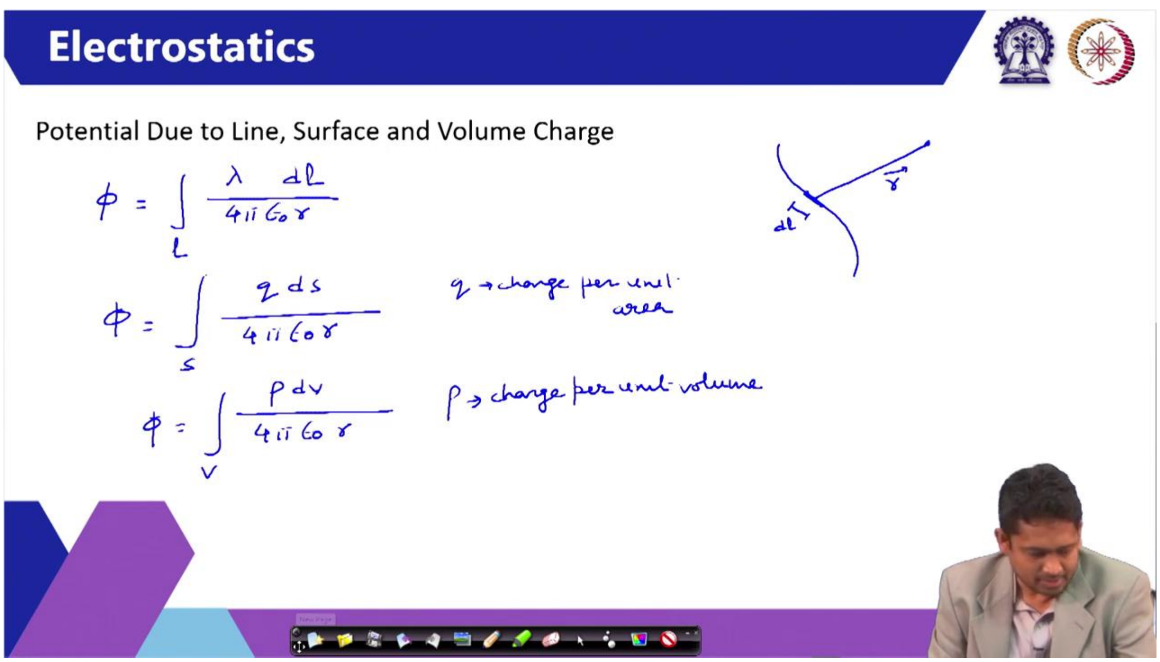

Now, we will talk about potential due to line surface and volume charges. So, let us imagine that we have a line over which charge is distributed and we want to find out electric field or potential here.

Now, let us imagine that we are taking a small segment of this line and let us call it dl and the vector that is joining this dl with this point is r. It is r vector. Now, this is a very small segment dl. So, that is why the vector joining the beginning of this segment with this point or the beginning of this segment with this point are almost same. Now, if that is so, we can define the potential as this.

$$\phi = \int_L \frac{\lambda}{4\,\pi\,\epsilon_0 r} dl$$

So, here the total charge in this segment is lambda dl. So, because of that the potential is lambda dl by four pi epsilon zero r and then if we integrate it over the line length, I mean the entire line there it is. We get the total potential here.

Now, similarly if there is a distribution of charge over a surface and that charge per unit area is q then we can rewrite the expression as - four pi epsilon zero r and accordingly where q is charge per unit area. So, q is charge per unit area.

$$\phi = \int_S \frac{q}{4\,\pi\,\epsilon_0 r} ds$$

Similarly, if there is distribution of charge over a volume and charge per unit volume is rho we can write this as simply this. So, rho is charge per unit volume.

$$\phi = \int_V \frac{\rho}{4\,\pi\,\epsilon_0 r} dv$$

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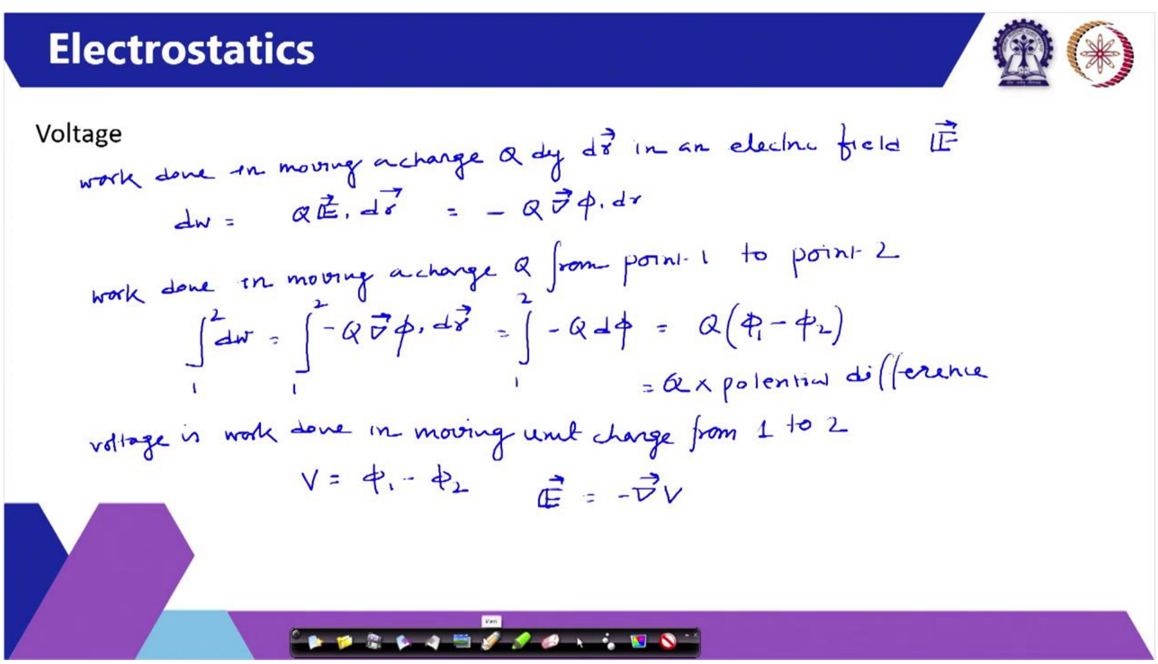

Now, we will go to another topic, I mean another definition and that is voltage. Now, voltage means work done on moving unit charge from one point to another point. So, first let us define work done in moving a charge Q by dr in an electric field E.

Let us define the dw. So, we are moving this charge by a small amount dr. So, as the amount is small, we can assume that along that small length, during that small displacement the electric field remains constant. So, the force is Q multiplied by E and that force dot dr is the amount of work done. Now, we know the relation between E, I mean electric field and potential. So, from that we can write this as this –

$$dw = Q\vec{\mathbb{E}} \cdot d\vec{r} = -Q\vec{\nabla}\phi \cdot d\vec{r}$$

Now, we just integrate it and find out work done in moving a charge Q from point 1 to point 2 and that becomes this. We just integrate dw over 1 to 2 and it takes this form. Now, del phi dot dr, this can be written as d phi and then this quantity on being integrated gives me Q multiplied by phi 1 minus phi 2. So, we have Q multiplied by potential difference.

$$\int_1^2 dw = \int_1^2 -Q\vec{\nabla}\phi \cdot d\vec{r} = \int_1^2 -Qd\vec{\phi} = Q(\phi_1 - \phi_2)$$

Now, as per our definition so voltage is defined as work done in moving unit charge from 1 to 2. So, that tells us that voltage is just phi 1 minus phi 2.

$$V = \phi_1 - \phi_2$$

And if we want to relate it with the electric field this gives us electric field is equal to minus of gradient of voltage.

$$\vec{\mathbb{E}} = -\vec{\nabla}V$$

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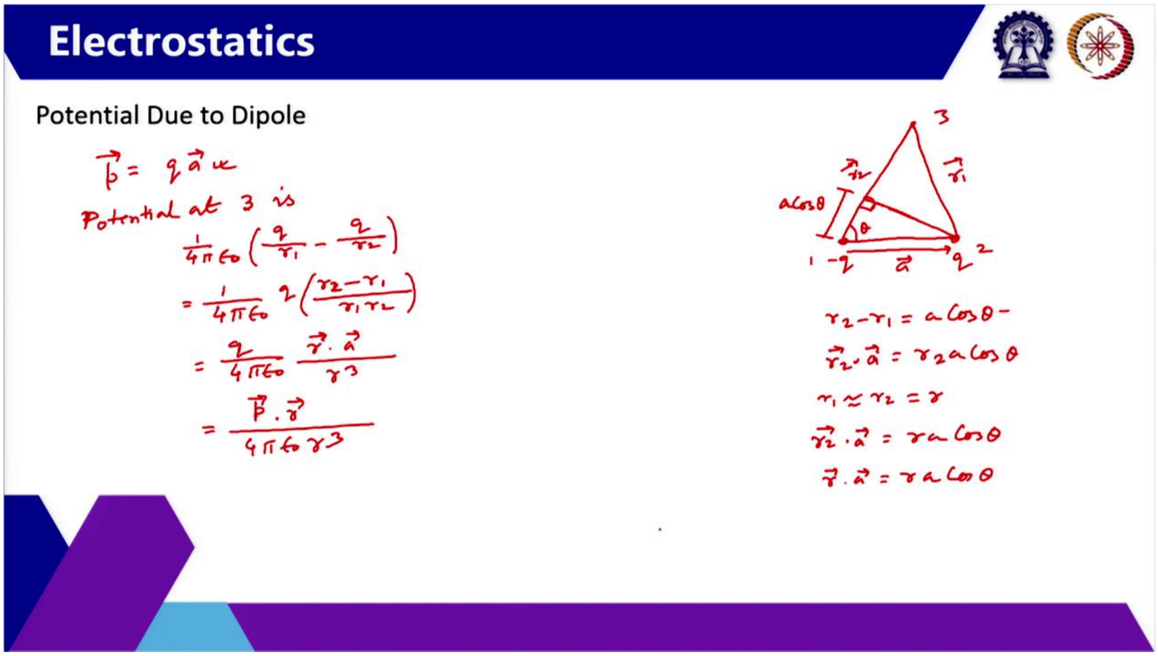

Now we will talk about potential due to dipole. So, let us imagine that we have 2 points, point 1 and point 2 with charge - q and + q and the vector from - q and + q is a vector. So, the dipole moment that is created is p is equal to q a.

$$\vec{p} = q\vec{a}$$

So, let us name them, point 1, point 2 and let us say that we are interested to find out potential at another point 3. Now if I join point 1 to point 3 and the corresponding vector is r2 and if we join point 2 to point 3, the corresponding vector is r1 and the angle between 1-2 and 1-3 is I mean the vector a and vector r2 is theta. So, potential at 3 is 1 by 4 pi epsilon then potential due to the positive charge which is q. So, q by r1 minus that due to the negative charge.

$$\frac{1}{4\pi\epsilon_0}\left(\frac{q}{r_1} - \frac{q}{r_2}\right)$$

Now we can write this expression as q multiplied by r1 minus r2 by r1 r2.

$$= \frac{1}{4\pi\epsilon_0} q \left(\frac{r_2 - r_1}{r_1 r_2}\right)$$

Now, let us put a perpendicular from point 2 to the line 1-3. So, this is a perpendicular. Then this becomes a cosine theta and this can also be written as r2 minus r1 is equal to a cosine theta.

$$r_2 - r_1 = a\cos\theta$$

And then we can say that r2 dot a is r2 a cosine theta.

$$\vec{r_2} \cdot \vec{a} = r_2 a \cos\theta$$

Now please understand that the distance between this positive and negative charge is much less than the distance 1-3 and 2-3 and that is why we could write this and again with that assumption r1 is equal to r2 is equal to r.

$$r_2 \approx r_1 = r$$

We can write r2 dot a is equal to r a cosine theta or r dot a is equal to r a cosine theta.

$$\vec{r_2} \cdot \vec{a} = ra\cos\theta$$

$$\vec{r} \cdot \vec{a} = ra\cos\theta$$

So, if we put all these approximations here. So this q then we can write, so this is r2 minus r1, not r1 minus r2 if I do the subtraction. So, then it becomes r dot a divided by r cube and we know that q multiplied by a is the dipole moment vector p.

$$= \frac{q}{4\pi\epsilon_0}\left(\frac{\vec{r} \cdot \vec{a}}{r^3}\right)$$

So, we can say p dot r divided by 4 pi epsilon r cube. So, that is the potential at point 3 due to the dipole.

$$= \frac{\vec{p} \cdot \vec{r}}{4\pi\epsilon_0 r^3}$$

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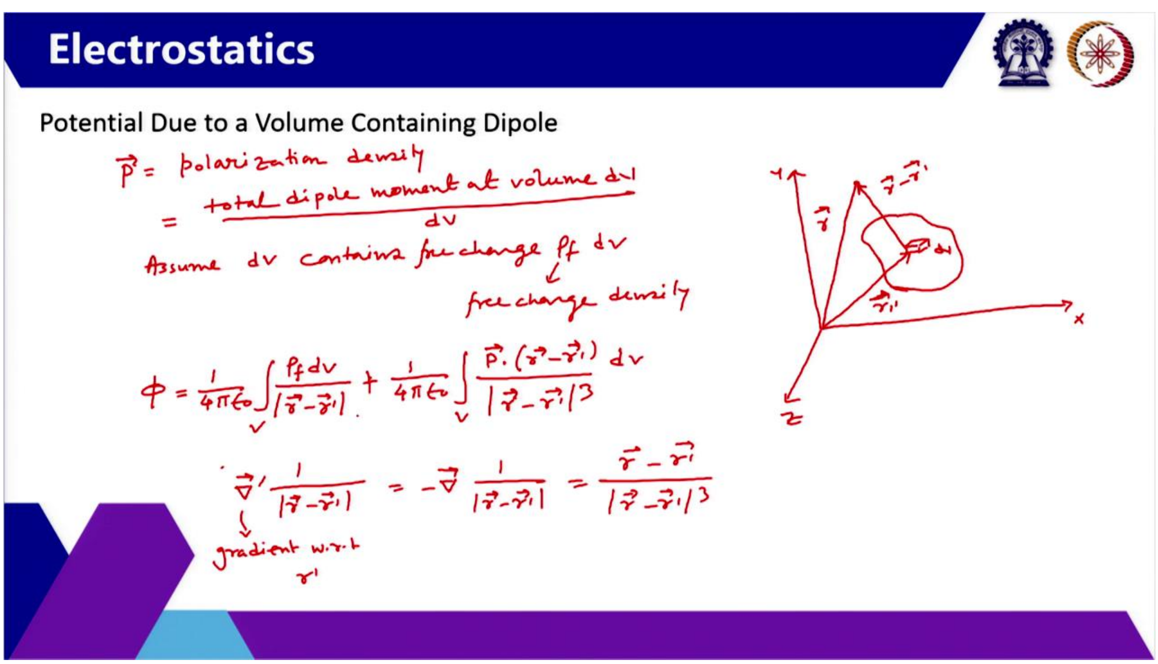

Now we will talk about potential due to volume with a dipole. So, let us imagine that we have a volume V that contains lot of these dipoles and free charge as well. We can say that for dielectric material free charge is 0, but let us have it for the time being we can always say later on that it is 0.

Now within this volume let us consider a small volume dV and the vector joining the origin to dV is r prime and let us say that we are interested in finding out the dipole at a point and the vector joining this is r. So, the vector that joins dV with our point of interest is r minus r prime. So, this is r minus r prime. Now let us define something called polarization density. Polarization density is total dipole moment at volume dV divided by dV and assumes dV contains free charge rho f dV where rho f is our free charge density.

Now with this we can say that the total potential at that point of interest is 1 by 4 pi epsilon 0, then our potential due to that charge which is rho dV divided by the magnitude of r minus r prime and dV is already there plus 1 by 4 pi epsilon 0. Then our total polarization at that volume dV is PdV and because of that the potential at our point of interest is this P dot r minus r prime divided by magnitude of r minus r prime cube of that.

$$\phi = \frac{1}{4\,\pi\epsilon_0}\int_v \frac{\rho_f}{\left|\vec{r} - \vec{r'}\right|}\,dv + \frac{1}{4\,\pi\epsilon_0}\int_v \frac{\vec{P}\cdot\left(\vec{r} - \vec{r'}\right)}{\left|\vec{r} - \vec{r'}\right|^3}\,dv$$

Now let us define a gradient vector with a prime. Gradient of r minus r prime. So, this gradient with a prime is taken, gradient with respect to r prime.

So, here we do the integral over dV. So, this small volume dV at x, y, z is going to change. So, if I take the gradient with respect to that let us denote this as gradient with a prime. That is equal to a gradient, if it is taken with respect to this point, our of interest with a minus of that. So, gradient with a prime is equal to minus of gradient without a prime when it is taken with respect to this point and that is equal to r minus r prime divided by r minus r prime magnitude of that with a cube.

$$\vec{\nabla'}\frac{1}{\left|\vec{r} - \vec{r'}\right|} = -\vec{\nabla}\frac{1}{\left|\vec{r} - \vec{r'}\right|} = \frac{\vec{r} - \vec{r'}}{\left|\vec{r} - \vec{r'}\right|^3}$$

So, now, this expression r minus r prime divided by the r minus r prime magnitude of that with cube, this we can replace by this gradient.

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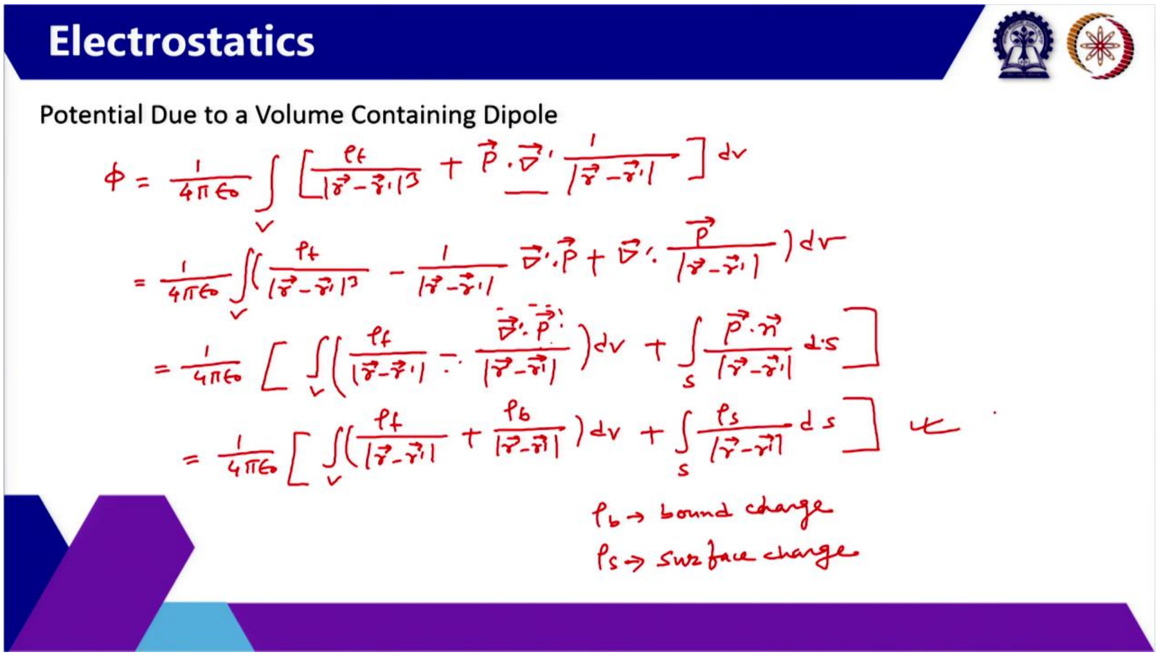

And after we do that it becomes phi is equal to 1 by 4 pi epsilon volume then we have rho f and cube of that plus P dot gradient with a prime of the magnitude of r minus r prime dV.

$$\phi = \frac{1}{4\,\pi\epsilon_0}\int_v \left[\frac{\rho_t}{\left|\vec{r}-\vec{r'}\right|^3} + \vec{p}.\vec{\nabla}'\frac{1}{\left|\vec{r}-\vec{r'}\right|}\right] dV$$

Then we can further do some manipulation, first term remains same. Now, this can be written as minus of delta dot P. So, here gradient with respect to a prime. So, plus delta prime dot this because we can always say that this gradient of P by mod of r minus r prime is equal to P dot gradient of 1 by mod of 1 minus r prime plus 1 by r minus r prime plus gradient of P. So, that is why we can rewrite this expression as this.

$$\phi = \frac{1}{4\,\pi\epsilon_0}\int_v \left[\frac{\rho_t}{\left|\vec{r}-\vec{r'}\right|^3} - \frac{1}{\left|\vec{r}-\vec{r'}\right|}\vec{\nabla'}.\vec{p} + \vec{\nabla}'\cdot\frac{\vec{p}}{\left|\vec{r}-\vec{r'}\right|}\right] dV$$

Now, if I further do this, then we get rho f minus dV. Now, this is a volume integral with a gradient. So, we can always write that as P dot n, n means normal to the surface and the surface integral. So, we convert this volume integral to a surface integral and write like this.

$$\phi = \frac{1}{4\,\pi\epsilon_0}\left[\int_v \left(\frac{\rho_t}{\left|\vec{r}-\vec{r'}\right|} - \frac{\vec{\nabla}'.\vec{p}}{\left|\vec{r}-\vec{r'}\right|}\right) dV + \int_S \frac{\vec{p}.\vec{n}}{\left|\vec{r}-\vec{r'}\right|} dS\right]$$

Now, this term has the same dimension as rho f. So, delta prime dot P has the same dimension of rho f. So, delta prime dot P with a minus can be called as rho b. So, we say rho f by plus rho b dV and this we give a name P dot n we give a name we call it rho s ds.

$$\phi = \frac{1}{4\,\pi\epsilon_0}\left[\int_v \left(\frac{\rho_f}{|\vec{r} - \vec{r'}|} + \frac{\rho_b}{|\vec{r} - \vec{r'}|}\right) dV + \int_S \frac{\rho_s}{|\vec{r} - \vec{r'}|}\, dS\right]$$

So, rho b we call a bound charge and rho s we called surface charge. So, we found out the expression for potential in due to a dipole continuum and while deriving this expression we got two more terms; one is a bound charge, one is a surface charge. We have a free charge also, but later on we can say that our free charge is 0. So, this is the total expression of potential due to a continuum containing dipoles.

So, with this I would conclude the lecture here.

Thank you.