Carbon Materials and Manufacturing
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Lecture - 02
Mathematical Representation of Material Properties

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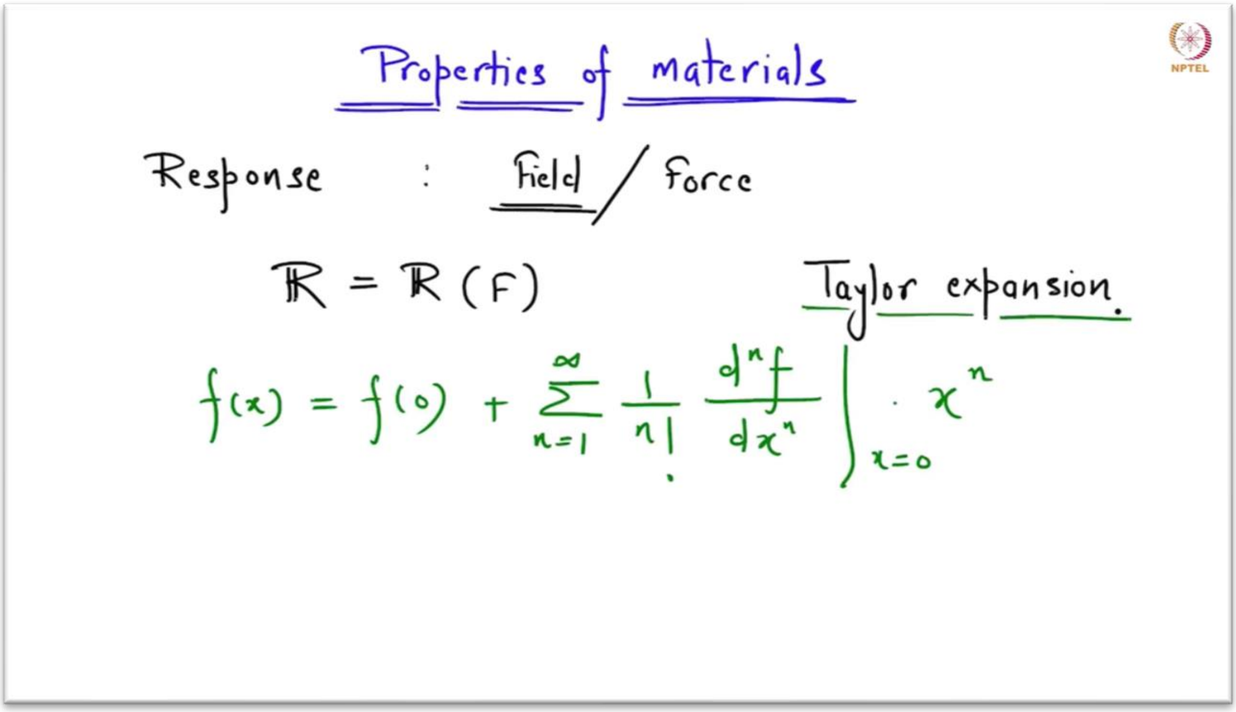

Ok so now, we are going to learn something very interesting. What are the properties of materials? If I ask you need to define all the properties of all the materials. What is the definition of the word ‘properties’ itself? Then what are you going to say? Ok, well you know that different materials behave differently under certain conditions, a specific set of conditions.

For example, I start heating a material. So, some materials will melt, some materials will conduct the heat, or some materials will not heat up at all, so there will be thermal insulators. Also, in a given range of temperature, you will have a different response from the material and then let us say if the temperatures are too high or too low, you may get a different type of response.

Similarly, for example, you know about stress or mechanical properties. In a certain range of forces or loads, you have a linear response from the material, where stress is proportional to the strain. But in another range, maybe the material will fracture, or the material will not behave linearly.

So, what is property again? Property is nothing but the response from the material. So, the response from any material to; what? To a certain field so let us say or to a certain force applied force. Now, we can have different types of forces; we can have electrical forces or magnetic forces. So, we would use the term field for all of these things. But let us say there is an external field now, my material gives a response R.

So, how do I define R? This R is a function of whatever external field you have applied. So, this is basically the definition of the property but let's get into a little bit more, because the response as I already told you may not always be linear. Also in different fields, you will have different kinds of responses, it may be linear in some range and may not be in the other range.

So, how do we expand something mathematically? One thing that comes to your mind something very simple is the Taylor expansion. So, I am going to write how do we do the Taylor expansion, although most likely you remember it. I am going to write for any given function say f(x), which is a function of x.

So, what is the simple expression for the Taylor series? We know that it is expressed as:

$$f(x) = f(0) + \sum_{n=1}^{\infty} \frac{1}{n!} \frac{d^n f}{dx^n}\bigg|_{x=0} \cdot x^n$$

So, this is your Taylor expansion you know, this is the Taylor series, this is your expression. Now let us try to also express our material response in terms of the Taylor expansion.

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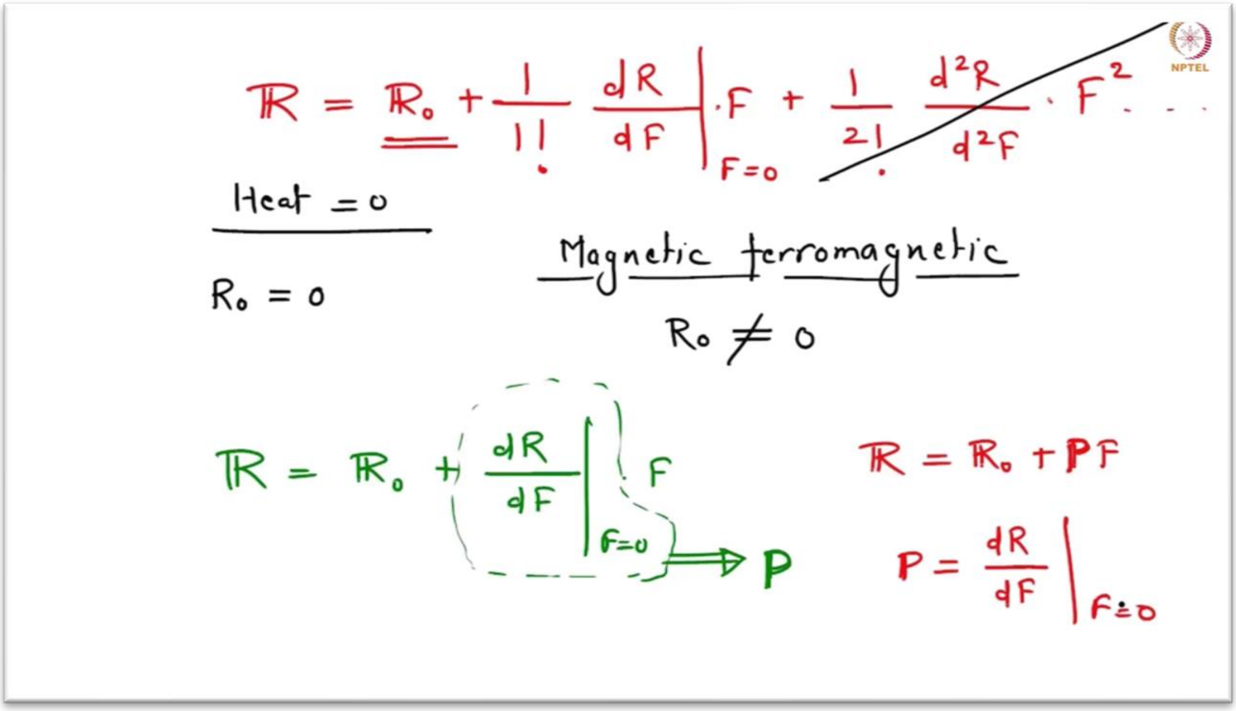

So, how do I write that? Let us say this is my response R(F). It will have some response R_0 without any external force or field, and then you can now write down a couple of terms. Let me write down let us say two or three terms using Taylor expression. So, I am assuming that my response does not depend on anything other than the field at this point.

$$\mathrm{R} = R_0 + \frac{1}{1!}\frac{dR}{dF}\bigg|_{F=0} \cdot F + \frac{1}{2!}\frac{d^2R}{d^2F}\bigg|_{F=0} \cdot F^2 + \cdots$$

So, this is your Taylor expansion of the response of your material. Now there are a couple of things here. First of all, before we get into the higher-order terms, let us see what is R_0. So, R_0 is nothing but the response of the material when the field equals 0. So, this is like the intrinsic property of your material. So, when do you have the intrinsic property?

Let us take a couple of examples. First, take the example of thermal conductivity. So, the thermal conductivity of the material will show the response only when the material heats up, which basically means that you need to provide some heat and so that is your field here. R_0 basically means your heat equals 0. So, you are not providing any external heat at that given point which basically would mean that there will be no response from the material. So, in this particular case, your R_0 is 0.

However, if we take another example, let us say the magnetic properties of iron or any ferromagnetic material. Then what happens is, even when there is no external magnetic field applied, there is some value there is some R_0 value is there, so it is a nonzero value. So, these are the two types of responses that you can get when there is no external field.

So, what we are going to do is, we are going to keep this particular term R_0, and then we will now move on to the higher-order terms. So, in this particular case, I assume that my material after the first order there is nothing. So, what do I mean by that? This is the first term basically is just your first linear response, but the second and higher-order terms basically show the non-linear behaviour of the material.

So, what I can do? I can rewrite this expression as:

$$R = R_0 + \left.\frac{\mathrm{dR}}{\mathrm{dF}}\right|_{x=0} F$$

So, this is the expression that basically now tells me what the material property is. You see that this $\left.\frac{\mathrm{dR}}{\mathrm{dF}}\right|_{x=0}$ term basically is the characteristic of my material. And this is what I can simply call the property of the material or let us say I have just written it is equal to P here.

$$P = \left.\frac{\mathrm{dR}}{\mathrm{dF}}\right|_{x=0}$$

What does this mean? So, now I will rewrite this term. So, I can say that my R basically equals whatever was the R_0 if it was a nonzero value plus P×F. So, this P now is the property. So, you will often see this kind of expressions in the case of the linear behaviour of the material.

So, if we do not go into the non-linear region. And then what is your property basically? Property is nothing but the response of your material with respect to a certain field when the field equals 0, the zeroth term basically. So, this is how you define the material property.

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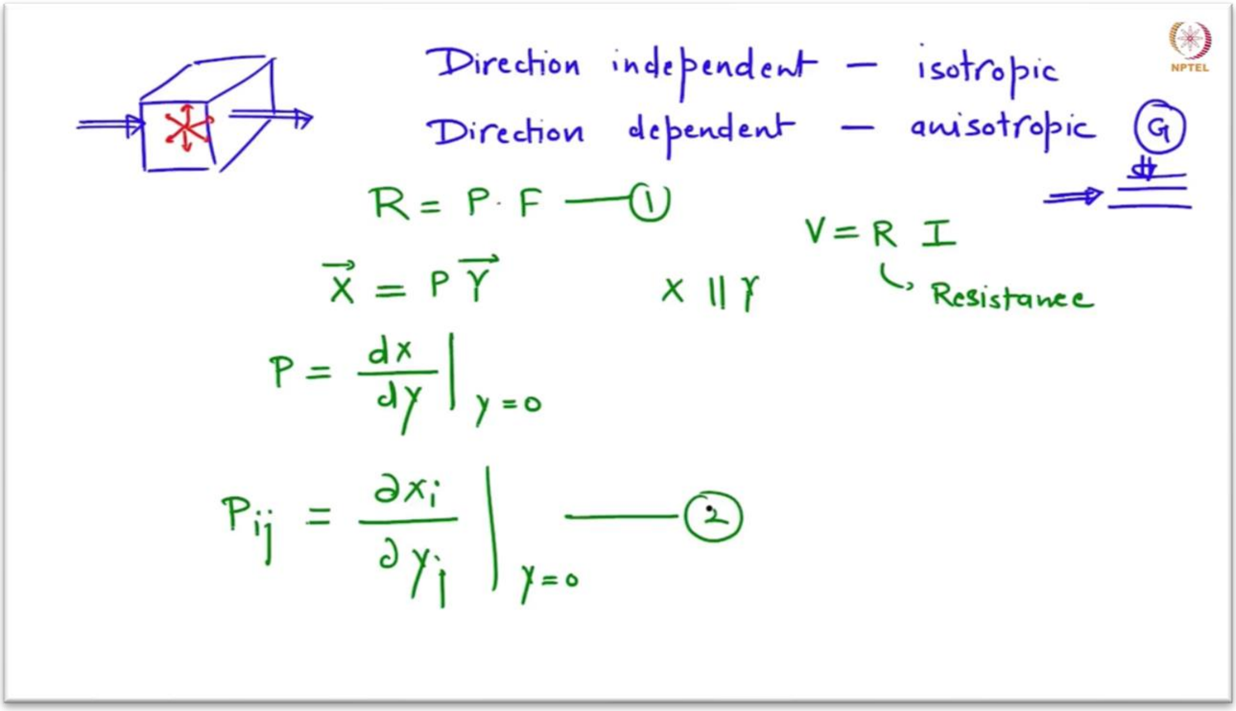

Now, the response from your material is same in all directions. So, if I have some crystal and I apply a certain force or an external electric field or if I provide heat, what is the response from your material? Is it same in all directions? or is it different in some directions and in different in other directions?

So, indeed there are both types of materials. The materials that offer the properties which are independent of directions. They are called isotropic materials, or the properties are also called isotropic properties sometimes.

And of course, then we also have other types of materials which will offer direction dependent properties. And why would that happen by the way? If you have a certain type of molecular structure or crystal structure, in that case what you will have is what is known as the anisotropic properties.

Now interestingly you will see the examples of both properties in our very interesting carbon materials, that we are going to learn most extensively in this course. Graphite that is a material which offers anisotropic properties because of its layered structure. So, if there is something with layered structure, if I apply a force from top or a force from the side, then I am going to get different kind of response from the material.

Similarly, this is also valid fo the electrical properties of the material or various other thermal properties. So, we are going to see both types of properties. Now, again how do you know? go back to you know mathematically describing these kinds of properties.

So, let us first you know go back to our usual expression. What was the expression again? We had,

$$\mathrm{R} = \mathrm{P} \times \mathrm{F} \tag{1}$$

And we can also find various examples of know this kind of expression. Let us say we talk about voltage and current. So, you know that voltage and current are proportional in any material, but there is some proportionality constant; in this particular case, this is the resistance.

So, electrical resistance is the intrinsic property or the characteristic of the material itself. So, this is a very simple example of linear response of the material, these kinds of expressions you have seen multiple times. So, in a more general form, let me write it as:

$$\vec{X} = P\vec{Y}$$

Till now, we have considered X and Y as scalar properties. So, basically there was no nothing to do with the directions, but it is also possible that it the properties or the material is anisotropic, which means that your X and Y both have some direction associated with them, and they are both now vectors. P still remains scalar because p in most cases is a number.

So, it is like electrical resistance. But if you have properties which are direction dependent in that case what happens? So, what is P by the way here? P in this particular case is:

$$P = \left.\frac{\mathrm{dX}}{\mathrm{dY}}\right|_{Y=0}$$

Now, if I have the direction dependent, in that case I will write:

$$P_{ij} = \left.\frac{\mathrm{d_i}X}{\mathrm{d_j}Y}\right|_{Y=0} \tag{2}$$

So, this is now going to the other expression for your property itself. Now, how many combinations are possible? Now, you have nine possible combinations of X and Y in the i and j directions.

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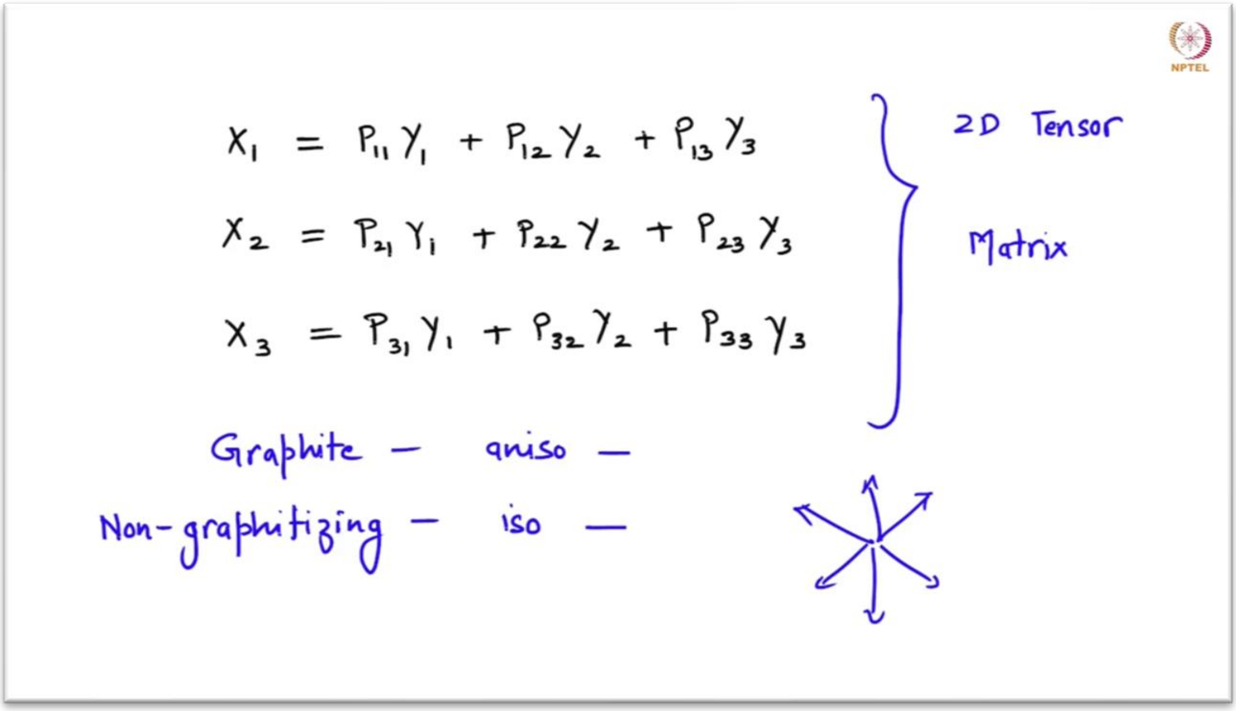

So, let me write down these expressions again.

$$X_1 = P_{11}Y_1 + P_{12}Y_2 + P_{13}Y_3$$

$$X_2 = P_{21}Y_1 + P_{22}Y_2 + P_{23}Y_3$$

$$X_3 = P_{31}Y_1 + P_{32}Y_2 + P_{33}Y_3$$

So, here I have written down all the expressions. These are the general expressions which can be represented as a 2D tensor or a matrix. So, now why we are discussing all this? Because in this particular course we are going to learn about a lot of carbon materials, I already told you that graphite has an anisotropic or direction dependent properties.

But there are also some carbon materials for example, something that we call as non-graphitizing carbon materials. they have their properties are isotropic, that means, they have their crystal structure such that whenever you apply any particular field, then you see the response in all directions.

And also, we may or may not be able to go into the details of the mathematical expressions every time, but I hope that from this lecture you will remember how to expand the properties of the material.

So, when we talk about the response R_0 is the term which is the residual or the permanent property that we have already learnt, and the first term then expresses the properties in the beginning of your experiment. So, when the field is just applied and that is why we call it field equals 0.