

**Nanotechnology Science and Applications**  
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**Lecture - 24**  
**Carbon Nanotubes**

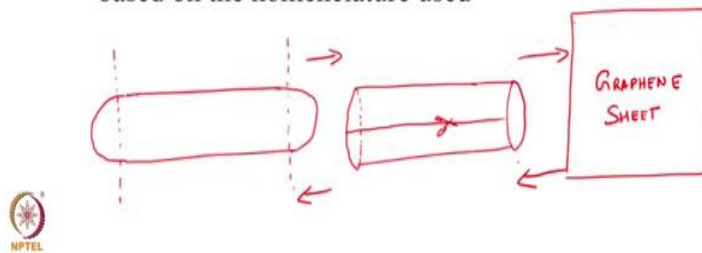
Hello in this class, we will look at one of the Nanomaterials that is derived based on carbon and that is the Carbon Nanotube. It has been around now, as a material of interest for almost now nearly 25 years maybe and people have been studying it and trying to use it for various applications.

So, today we will spend some time, looking at this material trying to understand certain aspects associated with it.

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### Learning Objectives

- 1) Explain the nomenclature used to describe carbon nanotubes
- 2) Derive important parameters of the nanotubes based on the nomenclature used



In particular, we will look at; we will explain some nomenclature. I will look at some nomenclature that is used with respect to carbon nanotubes because if you read publications in the area of carbon nanotubes, you will tend to see this nomenclature. So, we will explain, we look at that and I will try to explain what that nomenclature is and how it comes about. We will also derive some important parameters of the nanotube, particularly it is diameter and also how it is twisted things like that, based on the nomenclature used. So, this is the idea that we will look at this class and this is the set of learning objectives that we have for the class.

So, to begin with, we will start/a small rough diagram of what the nanotube is and I will show you what is it that we are going to do to put some numbers to this description.

So, the general description is that it is like a tube. So, you have a cylinder and then. So, this is like the you know if you have the tube and you take a section like this; this is what you would see, you would see a cylinder and then you would see some two end caps. So, this is what you are seeing it is a cylinder with the two end caps and I have taken a vertical section; so, you are sort of a cylinder that is lying flat on a surface and then I have taken a vertical section. So, you see a cross-section that looks like this.

Now we want to use, we want to say certain things about it; we want to say something about its diameter, we want to say something about how the carbon atoms are sort of lined up with respect to each other and so on. So, to do that, one of the ways in which we can do it is to first start with a single graphene sheet. So, a single sheet of graphene and then fold it to create this carbon nanotube.

So, I must point out that in the general synthesis of carbon nanotubes this is not the process that is actually used. We do not start with graphene sheets and then fold them to get the carbon nanotube in the actual typical experimental synthesis processes, that is used in the labs. Instead, we use certain processes that we will describe in a later class which helps us create the nanotube or synthesize the nanotube access. So, you get the nanotubes in its final form.

So, this is not how it is made, but this description if you look at it as a sheet that has been rolled to create the nanotube; then you are better able to understand how the structure of the sheet relates to the structure of the nanotube. So, that is what we will do.

So, if you take this tube for example, and you cut off the hemispherical ends. So, then you will have a hollow tube. So, you will have a tube-like that, simply a hollow tube. So, you have a hollow tube-like that; and then you can cut this tube and open it up. So, supposing I cut it like this. So, I snip it like that and then I open it up into a sheet, then I would get a sheet like that. So, I started with the tube, I cut off its end caps, then I arrived at a hollow tube and then I cut open that hollow tube and got a sheet.

So, this is the manner in which, I am explaining the arrangement of the tube and how it relates to the sheet. So, in reality, we could do the opposite. So, in fact, that is what we

are going to do in the class, we are going to take the sheet which is the graphene sheet, and then roll it to get the tube; so that is how you would get this tube. And then later we will look at the end caps; we are not going to look at the end caps immediately today, but we relate to look at how those end caps might come about. So, but you can see, how the graphene sheet when it is rolled will get you a tube

And in this process, we can understand how that rolling happened and how that tube came about; and how you can relate some things with the that relate to the structure of the graphene sheet to the structure of the tube. So, for example, I am now going to explain the same thing with a sheet of paper, which we will pretend for the moment is a graphene sheet. So, this is a sheet of paper, we pretend that this is a graphene sheet like the one that you see on the right extreme of your screen. And then you can see that I can actually roll it around; and once I have done rolling it around, I get a cylinder. So, I get a cylinder, a hollow cylinder is what I have. So, I can start with the sheet roll it around get a cylinder.

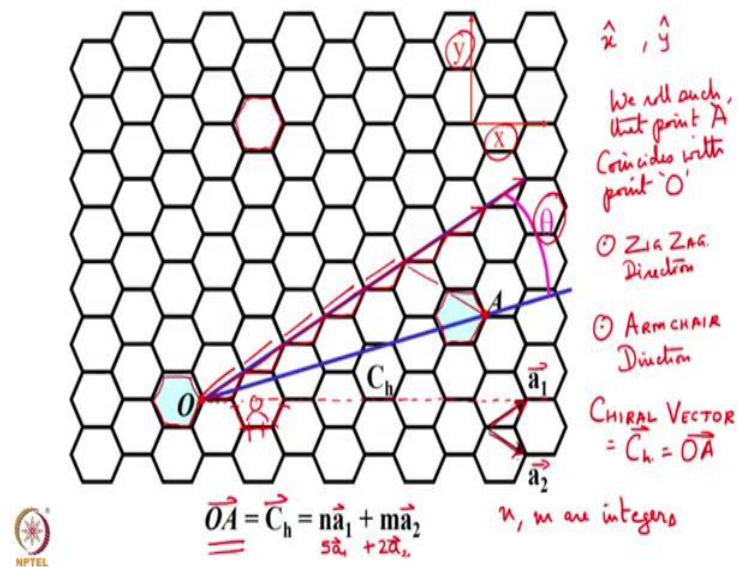
Now the interesting thing to note is that, when I say how the, when I make a mention of how the arrangement of atoms in the sheet relates to the tube; what I mean is although I have just rolled this to get you the tube, there is we have actually a few different options on how you can roll this to get the tube. So, this is one way in which you can get the tube, I can also twist the sheet when I roll it. So, in other words, I would twist it like this.

So, I twist it like this and I can still get a tube. So, I have now twisted it. So, I am still getting a tube, but it is not the same as the tube that we started with. So, this tube is not the same as what I previously showed you. So, this is a twisted tube. So, you can see here clearly it is a twisted tube, let me hold it correctly for you and show you. So, this is like a twisted tube. So, I can do it like this or I could do it like this. So, I can give it a twist.

So, this is called chirality and so, this is one of the things that we want to understand about the nanotube. We want to know whether the nanotube got formed like this or it got formed like that. So, and the reason we want to know is, it tells us something about the structural aspects of the nanotube. It also actually impacts very significantly on the properties of the nanotube; things like conductivity of the nanotube are often associated with the aspects of how it has being twisted. So, this is very important. So, knowing what

the chirality of the nanotube is and putting some kind of a number to it, some kind of numerical value to it gives us a better way of describing the nanotube and a better way of understanding what the nanotube is capable of. So, that, therefore, we are going to spend some time, figuring out how this structure relates to the nanotubes.

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So, what you see here is a graphene sheet. So, we will spend a few moments on this, we are going to derive things based on this. So, what do you see here are, so for example, this is all hexagonally bonded carbon atoms, the whole sheet consists of hexagonally bonded carbon atoms. So, I have just highlighted one of them, all. So, now, as I said one way to look at it, look at a nanotube is to roll, take a sheet-like this and roll it around and form a tube. So, now, we want to get a little bit more specific, on what have we done while we rolled it.

So, what we are saying is, let us look at two different hexagons here. So, one hexagon is here and another hexagon is here ok; and I identified two points this is O and this is A. Now the idea of saying, I know how I rolled it is basically translated to the sheet to say that, when I roll it, I get the point A to coincide with a point O. So, we roll such that point A coincides with point O.

So, therefore, now we have a much more specific way in which I specify that I have rolled the sheet. In other words, if you also take a sheet you have a separate graphene sheet and I have a separate graphene sheet; and if we are able to specify O and A like this

and then roll the sheet such that O coincides with A or A coincides with O. Then the two tubes that we will get will be identical; the tube that you get and the tube that I get will have the same kind of twist and therefore, many of the properties will start getting defined appropriately. So, this is the idea.

So, now, with respect to the graphene sheet, there are two directions that are defined; from the perspective of symmetry between these two directions, we have a range of possibilities and then outside of these two directions whatever you see, symmetry is the same as what you would see within these two directions. So, what are these two directions? One direction is referred to as the zigzag direction. So, one direction is referred to as the zigzag direction.

So, for example, you see this line marked here, this is the zigzag direction. So, as you can see it is easy to visualize it with respect to the graphene sheet structure, because basically you just see this, if you go along the direction you see the zigzag pattern right, it goes zigzag like that. So, therefore, you can visualize this direction as the zigzag direction. So, when I say zigzag direction you can quickly understand what exactly I am referring to. There is another direction which is in this direction here, this is dotted line that I am drawing; this has another descriptive way of being referred to and that is called the armchair direction.

So, the first one that I wrote there is the zigzag direction, and a second one that I have drawn here is the armchair direction. So, this is some general descriptive term that has been used in the literature. And why do we call it armchair? Well again there is no it is not a very scientific way of putting a descriptive name to this particular direction; but generally if you look at it if you consider this as the base of the chair and these as the two arms of the chair, you are such that you are going to be sitting on this place here like that.

So, then you can loosely say that this is described as an armchair and then this direction is then the armchair direction. So, these two would be considered the arms of the chairs and that is the chair. So, well you can argue that that is not a very great description, but that is the description that is used in the literature; and therefore, that is the armchair direction. So, this direction this dotted line that I have drawn here is the armchair direction.

So, what I have drawn here, OA. So, the vector OA, if you say O is the origin and A is another point there on this lattice; OA is a vector, this vector is somewhere between these zigzag directions and the armchair direction. And we have a choice a range of vectors like this that we can select, which all go between the armchair direction and the zigzag direction. And as I said because of symmetry if you go beyond this on either side, you are essentially repeating the same thing. So, therefore, it is sufficient that we look at the structure within the scope of this zigzag direction and the armchair direction.

So, now, we are basically saying that we have rolled the sheet so that A coincides with O. So, now, what we do is, we specify a few things here, we say that the angle that the vector OA makes with the zigzag direction is this angle  $\theta$ . So, this  $\theta$  is an angle that the vector OA makes with a zigzag direction. And we have the X and Y directions indicated here, X and Y direction. So, we will use unit vectors in the X-direction  $\hat{x}$  and unit vector in the Y direction  $\hat{y}$  to help us in some of these calculations.

So, we can also see here, I will put a vector here  $a_1$  and  $a_2$ ; these are the unit vectors of the graphene sheet, so  $a_1$  and  $a_2$ . And therefore, we can think of OA as it is called the chiral vector. So, it is called the chiral vector. So, this is the chiral vector Ch. So, I will put the vector or symbol here, is the vector OA. So, the vector OA is the chiral vector Ch. So, it is  $na_1+ma_2$ , so where n and m are integers.

So, for example, if you look at what do we mean/this, we have  $a_1$  direction here marked like this, you will notice that the  $a_1$  direction is exactly the same direction as the zigzag direction. So, the zigzag direction and the  $a_1$  direction coincide. So, when I say  $n \times a_1$  and  $m \times a_2$ ;  $a_1$  is this direction. So, we have to now have some combination of  $a_1+a_2$  which should get us to go from starting from O to arrive at A.

So, if you look at it here, I have to go 1 2 3 4 5. So, I have to travel 5 steps along the  $a_1$  direction, and I have to travel 2 steps along the  $a_2$  direction to arrive at A. So, I have to travel 5 steps in the  $a_1$  direction, two steps in the  $a_2$  direction to arrive at A. So, therefore, OA in this context is  $5a_1+2a_2$ .

So, in the context of this description, we are able to show that OA is  $5a_1+2a_2$ . So, in this case, n and m would be 5 and 2. Any other selection that you make, you will have a different value of n and different value of m. So, that is the way in which. So, almost all the tubes, the basically the tubes that you can generate using this sheet, can all be

described in terms of n and m. If what the n values and what the m value is you start, you will have a very good idea of what is the tube that you have created; and then from that we can ascribe properties to the tube.

So, this is what we will do, we will figure out some more properties of the tube-based on the values of n and the value of m. So, that is what our derivation in the rest of the class is going to be.

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$$|\underline{a}_1| = |\underline{a}_2| = a = 2.46 \text{ \AA} = \sqrt{3} a_{cc}$$

$$\underline{a}_1 = a \frac{\sqrt{3}}{2} \hat{x} + \frac{a}{2} \hat{y}$$

$$\underline{a}_2 = a \frac{\sqrt{3}}{2} \hat{x} - \frac{a}{2} \hat{y}$$

$$a_{cc} \frac{\sqrt{3}}{2} = \frac{1}{2} a \quad \therefore a = \sqrt{3} a_{cc}$$

$$\underline{C}_h = n \underline{a}_1 + m \underline{a}_2$$

$$\underline{C}_h = \frac{n a \sqrt{3}}{2} \hat{x} + \frac{n a}{2} \hat{y} + \frac{m a \sqrt{3}}{2} \hat{x} - \frac{m a}{2} \hat{y}$$

$$= \left( \frac{n a \sqrt{3} + m a \sqrt{3}}{2} \right) \hat{x} + \left( \frac{n a - m a}{2} \right) \hat{y}$$

So, now I have just magnified this  $\underline{a}_1$  and  $\underline{a}_2$  vector. So  $\underline{a}_1$  is there and  $\underline{a}_2$  is here and we have a unit vector in the X-direction which is  $\hat{x}$  and unit vector in the Y-direction which is  $\hat{y}$ .

So, this is basically you have two hexagons here. So, this angle is 120 this is also 120 and so is this. So, these three angles are 120°. So, if you see here, if you draw. So, if this is 120° angle. So, then you have 60° remaining. So, this is 30° and this is 30°. So, that is those are the angles of the triangle.

So, now let us see if you want to write  $\underline{a}_1$  in terms of unit vectors in the X direction and the Y direction. So, let us just see what that is. So, to do that I have to just draw the, extend it and draw like that and also draw it like this for  $\underline{a}_2$ . So, what do we have here, we have 30° here? So, if you see here, if I write  $\underline{a}_1$  modulus of  $\underline{a}_1$  equals the modulus of

$a_1$  equals some numerical value  $a$ ; then we have  $a_1$  is equal to  $a \cos 30$  which is  $\sqrt{3}/2$  in the x-direction  $+a \sin(30)$  which is half, so  $a/2$  in the y-direction.

$$a_1 = \sqrt{3}/2 \hat{x} + a/2 \hat{y}$$

So, you will have a  $\sqrt{3}/2 \hat{x}$  will bring you from here, from the origin to this point I have I will call it B, OB will move us in the X direction which is a  $\sqrt{3}/2 \hat{x}$ ; and then if I have to go from B to this point C then I have to do  $a/2 \hat{y}$ , so in the y-direction  $\hat{y}$  direction. So, this is  $a/2 \hat{y}$ . You will note that this is also  $a/2 \hat{y}$  and the and therefore, but except that this is in the negative direction. So, this is now we are talking of vector. So, this is in the negative direction.

So, if you write  $a_1$ , in the x-direction you travel the same distance a  $\sqrt{3}/2 \hat{x}$ ; but now in the y-direction, you are going in the opposite way like this as suppose to previously you went upwards, now we are going downwards. So, this is  $- a/2 \hat{y}$ . So, this is the way we write  $a_1$  and  $a_1$ . And incidentally these two if you just see, I have also written here that it is equal to  $\sqrt{3}a_{cc}$ . So, why does that come about  $a_{cc}$  is this bond length. So, from here to here, for example, this is  $a_{cc}$  and that is the same for all sides of the hexagon. So, all sides of the hexagon is equal to  $a_{cc}$ . So, that is the same as this distance marked here, from here to here is  $a_{cc}$ .

So, if you look at it, if you want to again look make draw a perpendicular bisector to that line, it will come here. So, this is  $30^\circ$ . So, whatever is the  $a_{cc} \times \cos 30$  which is  $\sqrt{3}/2$  is equal to half of; so because you have taken a perpendicular bisector here. So, this distance here is only half the value of a equal to half of a. Therefore, a is equal to  $\sqrt{3} a_{cc}$  and that is what I have put here. So, this is how they relate to each other and as necessary we will take this value and put it.

So, now if you go back to what we had for the chiral vector; we wrote the chiral vector equals  $na_1+ma_2$ . So, we will write

$$C_h = na_1+ma_2$$

Now we already have expression for  $a_1$  and we have an expression for  $a_2$ . So, we can substitute in this chiral vector notation and what will we have, we will have  $C_h$  equals  $na_1 + m(\sqrt{3}/2\hat{x} + a/2\hat{y})$  now, so that covers our  $a_1$  term,  $a_2$  term is covered; now we look at the  $a_1$



term here, that is  $m$ , so  $ma\sqrt{3}/2\hat{x}$ . So, because now we are going to do  $a_1$  we are take the second equation here, is this equation we have to take and multiply it/ $m$  and; so  $-ma/2\hat{y}$ .

So, now if we club together the terms in the X direction and terms in the Y direction; so, after we club them together, you will basically have

$$C_h = na\sqrt{3}/2 + ma\sqrt{3}/2\hat{x} + na/2 - ma/2\hat{y}$$

So, this is our chiral vector. So, in terms of in the taking some vectors in the X direction and Y direction, unit vectors in the X direction and unit vector in the Y direction clubbing the terms together for  $a_1$  and  $a_1$  you arrive at this value for the chiral vector.

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$|a_1| = |a_2| = a = 2.46 \text{ \AA} = \sqrt{3} a_{cc}$   
 $\vec{a}_1 = a \frac{\sqrt{3}}{2} \hat{x} + \frac{a}{2} \hat{y}$   
 $\vec{a}_2 = a \frac{\sqrt{3}}{2} \hat{x} - \frac{a}{2} \hat{y}$   
 $\vec{OA} = \vec{C}_h = n\vec{a}_1 + m\vec{a}_2$   
 $\vec{C}_h = \left( \frac{na\sqrt{3} + ma\sqrt{3}}{2} \right) \hat{x} + \left( \frac{na}{2} - \frac{ma}{2} \right) \hat{y}$

So, having done that, so this is what we have done here. So, you can see the same thing that, I put in the previous slide is what I have put down here. So, you can see this equation here and the second equation out here; those are the two equations that we have here.

Of course, we put the vector symbol here. So, this is  $x\hat{x} + y\hat{y}$ . So, therefore, we get this thing and we put this  $C_h$  equation also down, which we had here. So,

$$C_h = na_1 + ma_2 = (na\sqrt{3}/2 + ma\sqrt{3}/2) \hat{x} + (na/2 - ma/2) \hat{y}$$

so we got the expression for the chiral vector.

Now having got the chiral vector we would like to find two other parameters associated with the nanotube. So, what are the two parameters, we would like to understand, what is the diameter of the tube in terms of  $n$  and  $m$ ? So, in terms of  $n$  and  $m$  what is the diameter of the tube. So, that is one thing that we would like to derive; the other thing is in terms of  $n$  and  $m$ , we would like to understand, what is the theta to which we have twisted the tube? So, as I told you, you can join it like this or you can join it like that. So, that twist the chiral angle, it is called the chiral angle  $\theta$ . So, we would like to understand what is that value  $\theta$ , in terms of  $n$  and  $m$ ? And you also want to understand, what is the value of the diameter of the tube in terms of  $n$  and  $m$ ?

So, again if you look at it if you go back to how we had put this image together you can see here, that once you fold, so if you take the, if I say that I am going to roll the tube such that O and A coincide. So, then what is the meaning of that? The meaning of that is the line that goes from O to A is the circumference of the tube. So, if I have taken a point O I mean a point O here and a point A here and I roll it such that that O coincides with A.

So, I have got O to coincide with A, as I formed the tube. Then the OA vector basically goes from here, goes all the way around and comes back here. So, that is what that OA vector is. So, therefore, the chiral vector or rather the magnitude of the chiral vector is essentially the circumference of the tube. So, a magnitude of the chiral vector is the circumference of the tube and if you look at any and since the tube is circular in geometry; if you take the diameter of the tube to be  $D$  then  $\pi D$  is the magnitude of the circumference.

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$|a_1| = |a_2| = a = 2.46 \text{ \AA} = \sqrt{3} a_{cc}$   
 $OA = C_h = na_1 + ma_2$   
 $\vec{C}_h = \left( \frac{\sqrt{3}na + \frac{\sqrt{3}}{2}ma \right) \hat{x} + \left( \frac{n}{2}a - \frac{m}{2}a \right) \hat{y}$   
 $|\vec{C}_h| = \sqrt{\frac{3}{4}n^2a^2 + \frac{3}{4}m^2a^2 + 2 \times \frac{3}{4}nma^2 + \frac{n^2}{4}a^2 + \frac{m^2}{4}a^2 - \frac{2nm}{4}a^2}$   
 $= \sqrt{n^2a^2 + m^2a^2 + 2 \left( \frac{1}{2}nm \right) a^2}$   
 $= a \sqrt{n^2 + m^2 + nm} = a_c \sqrt{3(n^2 + m^2 + nm)} = \pi D$

So, therefore, essentially, we are saying that the magnitude of the chiral vector equals  $\pi \times$  diameter of the nanotube.

So, now we see that we have suddenly, we were looking at vector on a flat sheet of paper, we rolled it up to get the tube, and now we are able to relate the diameter of the tube to the magnitude of the vector when it was a flat sheet. We have also got an expression for the chiral vector as it is. So, we can use that to complete this calculation. So, that is exactly what we will do now. So, we have

$$C_h = (\sqrt{3}/2na + \sqrt{3}/2ma) \hat{x} + (n/2 a - m/2 a) \hat{y}$$

So, now, what is the modulus of  $C_h$ , it is simply the  $\sqrt{a_2^2 + b^2}$  that is basically the modulus; so, if the  $\sqrt{\text{this term, } a_2 \text{ of this term} + \text{the } 2 \text{ of this term}}$ .

So, this is equal to simply the square root of the two of this term plus the two of that term. So, if you take the two of this term the first term. So, you will get

$$C_h = 3/4 n^2 a_2 + 3/4 m^2 a_2 + 2 \times 3/4 n m a_2 + n^2/4 a_2^2 + m^2/4 a_2^2 - 2 n m/4 a_2.$$

So, this is the 2 of all the terms in this second part and this is the 2 of all the terms in the first part, of this part. So, this is what we have. So, now, we simply just simplify this and see what we have. So, we have  $n^2 a_2$  here. So, we have an  $n^2 a_2$  term here and you also have an  $n^2 a_2$  term here. So, this is  $3/4 n^2 a_2$  that is  $+1/4 n^2 a_2$ . So, that is  $n^2 a_2$ .

So, this is  $2\sqrt{n^2} a_2$  plus similarly you have a  $3/4 m^2 a_2$  here and  $a+1/4 m^2 a_2$  here. So, if you add them you have  $m^2 a_2$ . Then we have  $2 \times 3/4 n m a_2 - 2 \times n m/4 a_2$ . So, if you just simplify that is  $+2$  into  $3/4 - 1/4$  which is  $1/2 n m$ , and the whole thing is multiplied  $/a_2$ . So, therefore, if you simplify this further, you will simply have if you can pull out the  $a_2$  and then it is  $\sqrt{a_2}$ . So, it is  $a$ . So, this is simply  $a \times \sqrt{n^2+m^2+nm}$  is that right,  $2 \times 3/4 - 1/4$  will get you half. So, you will have  $n m$ . So, this is what you will get  $n^2+n^2+nm$ . So,  $a$  is out here.

And we also see that  $a$  is equal to  $\sqrt{3}a_{cc}$ . So, you can also write this as  $a_{cc}$  into  $3 \times n^2+m^2+nm$ . So, you can either write it using  $a$  or  $a$  that I have put here or you can write using  $a_{cc}$ .

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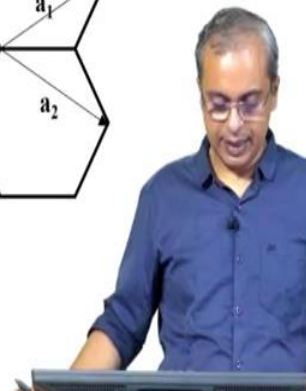
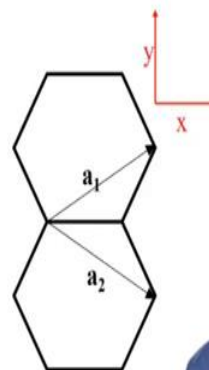
$$|a_1| = |a_2| = a = 2.46 \text{ \AA} = \sqrt{3} a_{cc}$$

$$OA = C_h = na_1 + ma_2$$

$$D =$$

$$\pi D = a \sqrt{3(n^2+m^2+nm)}$$

$$\therefore D = \frac{a_{cc} \sqrt{3(n^2+m^2+nm)}}{\pi}$$



So, this is the modulus of the chiral vector and this is equal to  $\pi D$ . So, therefore, so we can write that here, again  $\pi D$  equals you have  $a \times \sqrt{3(n^2+m^2+nm)}$ . Therefore, the diameter  $D$  of the nanotube relates to the values of  $n$  and  $m$  as I am sorry this is  $a_{cc}$  here. So,

$$D = a_{cc} \sqrt{3(n^2+m^2+nm)} / \pi$$

So, therefore, we find that we can actually start with  $n$  and  $m$  values. So, if you see here, you will see that down here as well; we will again come to that in just a moment. But you can see that, we have started with looking at the diameter of the tube; we looked at how the diameter of the tube of course because it is a tube  $D$  it has a circular cross-section and therefore,  $\pi \times$  the diameter of the tube is that circumference. And we also saw

the way we defined the tube, the way we created the tube; so, to speak conceptually was to take the circumference and roll it and that circumference there was the chiral vector,  $C_h$  or  $OA$  in this case. And therefore, we equated the magnitude of the chiral vector to the diameter of that to  $\pi \times$  the diameter of that tube; and then we did the mathematics and simplified it to see, how you could go from the chiral vector and related to  $\pi D$  and then arrive at a value for  $D$  in terms of  $n$  and  $m$ , because the chiral vector itself was described in terms of  $n$  and  $m$ .

So, this is what we got and that is what you see in your next slide.

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$$|\vec{a}_1| = |\vec{a}_2| = a = 2.46 \text{ \AA} = \sqrt{3} a_{cc}$$

$$\vec{OA} = \vec{C}_h = n\vec{a}_1 + m\vec{a}_2$$

$$\vec{C}_h = \left( \frac{na\sqrt{3}}{2} + \frac{ma\sqrt{3}}{2} \right) \hat{x} + \left( \frac{na}{2} - \frac{ma}{2} \right) \hat{y}$$

$$|\vec{C}_h| = \pi D$$

$$D = \frac{a_{cc} \sqrt{3(n^2 + m^2 + nm)}}{\pi}$$

You can see, we did all this, we wrote the chiral vector. So, I will put that down here. So, this is the modulus of  $a_1$  modulus of  $a_1$  is  $a$ ; and that is how they relate and the chiral vector  $C_h$  is  $n \times a_1 + m \times a_2$ . And that is how since we know what is  $a_1$  and  $a_2$  in terms of  $a$  and  $n$  and  $m$ , we arrive at these values for the chiral vector. And then once you take the modulus of the chiral vector and equate it to  $\pi D$ , we arrive at this equation here, which is what we did just a moment ago; on how the diameter of the nanotube relates to the values of  $n$  and  $m$  which then design, which are based on again how the tube has been created in terms of a twist in the carbon nanotube.

So, therefore, the  $n$  and  $m$  they are very useful in telling us what the diameter of the tube is. So, what we will do now is, this is one part of it, we would also like to see if you go back the other parameter that we want to get a handle off. So, we have now understood

how O A, how the value OA gives us the diameter D. We are also interested in this  $\theta$  value, the chiral angle. So, chiral vector and chiral angle are two important the parameters of a nanotube. We saw the chiral vector now Ch and we did certain calculations with respect to Ch; we would also like to do some calculations to get ourselves a value of  $\theta$  based on, what the chiral vector is.

So, if you see here, if you look at what we are dealing with here; if you take that  $a_1$  vector here, which is what is this vector here  $a_1$ . If I take a dot product of  $a_1$  and the chiral vector Ch, if I take a dot product of those two, then that is simply the magnitude of  $a_1$  into the magnitude of the chiral vector multiplied/cos of the angle between them.

So, the dot product of  $a_1$  and that cos of the angle that angle is this chiral angle. So, a dot product of the  $a_1$  vector with the chiral vector is simply the modulus of  $a_1 \times$  the modulus of the chiral vector  $\times$  cos of the angle  $\theta$  between them which happens to be the chiral angle. So, that is the approach we will use, we will use that equation and simplify that equation to arrive at the angle  $\theta$ . So, that is what we will do. So, if you go back, we will go to a place where we can do that for ourselves, so, the angle  $\theta$ .

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Diagram illustrating the chiral vector  $C_h$  and the lattice vectors  $a_1$  and  $a_2$  in a hexagonal lattice. The chiral angle  $\theta$  is shown between  $a_1$  and  $C_h$ .

Handwritten mathematical derivations for the dot product of  $C_h$  and  $a_1$ :

$$\vec{C}_h \cdot \vec{a}_1 = |\vec{C}_h| |\vec{a}_1| \cos \theta$$

$$= \left( \frac{\sqrt{3}na^2}{2} + \frac{ma^2}{2} \right) \cdot \left( \frac{\sqrt{3}na^2}{2} + \frac{ma^2}{2} \right) \cos \theta$$

$$= \left( \frac{3na^2}{4} + \frac{3ma^2}{4} + \frac{na^2}{4} - \frac{ma^2}{4} \right) \cos \theta = \left( na^2 + \frac{ma^2}{2} \right) \cos \theta$$

So, what is the angle  $\theta$ ? We are basically saying if you take the chiral vector Ch, I will remove this and your dot do a dot product with  $a_1$ , the vector  $a_1$  this is equal to modulus of Ch into modulus of  $a_1$  into cos of the angle  $\theta$  between them. So, we will use this process to arrive at our result. So, what is the chiral vector here? The chiral vector

$$Ch = na\sqrt{3/2} \hat{x} + ma\sqrt{3/2} \hat{y} \text{ also } \hat{x} + na/2 \hat{y} - ma/2 \hat{y}$$

this is the chiral vector. And the vector  $a_1$  itself we have derived defined it here. So, if you go back here you can see how we have defined the vector  $a_1$  it is defined here. So, we will use the same definition in our activity here. So, we will do a dot product of  $\sqrt{3/2} \hat{x} + \sqrt{3}a/2 \hat{y}$  then and  $a/2 \hat{y}$ . So, this is our dot product.

So, now, we simply have to do complete this math. So, what do we have here, you will see that if you take this term here, and you do a dot product with this term here; and correspondingly you take this term here and you do a dot product with this term here? So, we will have, let us see if you have some space here to do that. So, you will basically have. So, you take  $\sqrt{3}a/2$  and you do this you will have  $na_2/4 + 3ma_2/4$ . So, that is what you get  $3na\sqrt{3/2} \sqrt{3/2} + 3ma_2/4$  will go  $+3ma_2/4$ . So, we will have a

$$3na_2/4 + 3ma_2/4 + na_2/4 - ma_2/4$$

So, this is what we will have, when once we get done multiplying these terms. So, you will have  $na_2$  is what you will have here  $-ma_2/2$ . So, this is what we get as the dot product of  $Ch$  and  $a_1$ . And this we are going to equate to the modulus of  $Ch \times$  the modulus of  $a_1 \times \cos \theta$  it is. So, this is what we are planning to do. And if you see here the modulus of  $a_1$  and  $a_1$  is itself  $a$ . So, it is simply a value  $a$  is what the modulus is. So, that. So, this part is already known here this is the modulus of  $a$  and this is equal to  $a$ . So, we only need this modulus of  $Ch$ .

So, to get the modulus of  $Ch$ , we simply have to look at what we have here, we see that the  $Ch$  is this term that we have got out here; the  $Ch$  modulus of  $Ch$  we have already calculated here, this is the value that we got out here, this is the value of modulus of  $Ch$ .

So, this term also we have, modulus of  $Ch$  we have. So, therefore, if you go back to this equation we have here, this part that we have here is simply  $a \times \sqrt{(n^2+m^2+nm)} \times a \times \cos \theta$ . So, this is  $a^2 \sqrt{(n^2+m^2+nm \cos \theta)}$ . So, that is the right-hand side of this equation, this term here is exactly what this term here is and then we also found the left-hand side of this equation is here. So, we are only simply equating these. So, you are going to have. So, this is equal to  $n - m/2$  or  $2n - I$  am sorry this will be  $a +$  here; so,  $na_2 + m a_2/2$ . So,  $2n + m/2$  is what into  $a^2$ , is what this equation is and then this is equal to the term above.

So, this is the left-hand side of this equation here and what you see here is the right-hand side of this equation. So, these two are equal. So, now, if you equate these two, you can get  $\cos \theta$  very easily. And so, therefore, we will see that in our next slide.

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$OA = C_h = na_1 + ma_2$   
 $a_1 \cdot C_h = |a_1| |C_h| \cos \theta$   
 $\cos \theta = \frac{2n + m}{2\sqrt{n^2 + m^2 + nm}}$

$\therefore \cos \theta = \frac{2n + m}{2\sqrt{n^2 + m^2 + nm}}$   
 Diameter D  
 Chiral angle  $\theta$

We are simply going to write here, we are going to write  $a_2$  into  $2\sqrt{n^2+m^2+nm}$  is equal to, if you go back to the previous slide you will see the, I into  $\cos \theta$  is equal to  $2n + m/2a_2$ . So, this is what we have. So, now, we just have to simplify this you cancel the  $a_2$  and  $a_2$ ; therefore,

$$\cos \theta = \frac{2n + m}{2\sqrt{n^2 + m^2 + nm}}$$

So, this is the expression that we are getting here. So,  $\cos \theta$  is what we have here, is in the numerator  $\frac{2n + m}{2\sqrt{n^2 + m^2 + nm}}$ .

So, this is how we have got this equation. So, now, you see that the  $\theta$  value, which is basically this chiral angle here;  $\cos \theta$  is also related to the values of  $n$  and  $m$ . So, once the values of  $n$  and  $m$ , you can actually tell something about the  $\theta$  associated with this the nanotube; you can also say something about it is diameter. So, both these important things the diameter  $D$  and chiral angle  $\theta$ ; both of these we are able to associate with the values of  $n$  and  $m$ . We just doing some little bit of mathematics and calculating out  $a_1 \cdot C_h$  and then equating it to the modulus of  $a_1 \times$  the modulus of  $C_h \times \cos \theta$ .



So, once you do that, you get this equation. So, therefore, you can get all these parameters of the nanotube from  $n$  and  $m$  values; and that really is the primary idea that I wanted to discuss and elaborate upon in this class.

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### Conclusions

- 1) The notation  $n,m$  is used to describe different types of carbon nanotubes
- 2) When  $n$  and  $m$  are not equal, the nanotube is chiral
- 3)  $n, m$  can be related to the chiral angle
- 4)  $n, m$  can be related to the tube diameter



So, if you look at what we see here as our major conclusions; there is a notation  $n$  and  $m$ , that is used to describe different types of carbon nanotubes. So, we will see here that, there are carbon nanotubes that are referred to as zigzag carbon nanotubes; there are other carbon nanotubes that are referred to as armchair nanotubes, and there are carbon nanotubes which are referred to as chiral nanotubes, it is all got to do that angle of chirality, we will see that in our subsequent class.

So, the angle of chirality decides whether it is a zigzag nanotube, armchair nanotube or a chiral nanotube and therefore, this  $n$  and  $m$  is very useful in describing that. And when  $n$  and  $m$  are not equal, the nanotube is chiral or there are some specific values that the or at least especially if it is, you know; if  $m$  is not equal to 0 and then you have a range of values for  $m$  which are not equal to the value of  $n$  then it is referred to as chiral nanotube. And the values of  $n$  and  $m$  can be related to the chiral angle of the nanotube. And the values of  $n$  and  $m$  can also be related to the tube diameter.

So, therefore, in the context of describing nanotubes, if you use this description using the value of  $n$  and  $m$ , you can actually tell lot of things about the nanotube. It turns out that based on the values of  $n$  and  $m$ , things like electronic properties of the nanotube get fixed

or at least they tend to be a certain type. And therefore, it is very important, it is not simply a structurally descriptive approach which itself would be very useful; given that it is a tube and you are trying to explain something about the way in which the tube has been put together so that itself would be any way useful.

In this case, it also reflects very specifically with respect to the properties of the tube; and therefore, that is very important and therefore, this description is used. And we will see all those descriptions and how it relates to the properties in our subsequent class. So, with this we will halt for today.

Thank you.