

**Carbon Materials and Manufacturing**  
**Prof. Swati Sharma**  
**Department of Metallurgy and Material Science**  
**Indian Institute of Technology, Mandi**

**Lecture – 56**  
**Numerical Problems: Carbon Manufacturing and Characterization**

(Refer Slide Time: 00:13)

स्वाति शर्मा, भारतीय प्रौद्योगिकी संस्थान मण्डी

**Problem Set**




1. Calculate the required quantity of isotopically pure barium carbonate ( $\text{Ba}^{14}\text{CO}_3$ ; m. wt. 199) for achieving 1 millicurie activity.
2. Calculate the equilibrium reaction constant for graphite to diamond conversion at STP, if the energies of formation of diamond and graphite are 2.9 and 0 kJ/mol respectively. Mention the feasibility of the reaction at STP.
3. Calculate the boundary layer thickness inside a CVD chamber of 1 m diameter, where a hydrocarbon gas of density  $0.658 \text{ kg/m}^3$  and viscosity 0.55 poise is undergoing thermal decomposition onto a substrate of length 2 cm with a gas flow rate of 10 m/s.
4. Calculate the UV exposure time for a  $20 \mu\text{m}$  thick resist film on a silicon wafer, if the energy required for crosslinking is  $200 \text{ mJ/cm}^2$ .  
Given the lamp intensity is  $8.2 \text{ mW/cm}^2$ .



Hello everyone. In this lecture or let us say this is a tutorial, we are going to solve some mathematical problem, some numerical problems. During the class itself we have solved some problems, but I thought that some more examples are going to help you. Now, you can pause the video and or take a screen shot and go through these problems and then I am going to show you how to solve them.

(Refer Slide Time: 00:40)

Radiocarbon Decay law  $N = N_0 e^{-\lambda t}$    $N = \# \text{ unchanged @ } t$   
 $t_{1/2} = 5745 \text{ yrs.} = \frac{0.693}{\lambda}$   $N_0 = \# \text{ atoms @ } t$   
 $\lambda = \frac{0.693}{5745 \times 365 \times 24 \times 60 \times 60} \approx 3.83 \times 10^{-12} \text{ s}^{-1}$   
 $\# \text{ atoms decaying} \propto \# \text{ atoms present}$   
 $-\frac{dN}{dt} = \lambda N = \lambda \frac{W}{199} \cdot 6.023 \times 10^{23}$   
 $\approx 1.16 \times 10^{10} \cdot W \text{ s}^{-1}$

So, now, we are going to briefly or quickly solve our numerical problems. You can see the problem statements on the slide in the beginning. This is the one on radio carbon. You already know that what is the radioactive; decay law we also discussed and we also solved a little problem during the lecture.

The decay law basically states

$$N = N_0 e^{-\lambda t}$$

$N$  is the number of unchanged atoms at any given time  $t$ ,  $\lambda$  is your decay constant and  $N_0$  equals the number of total number of atoms at any given time  $t$ .

First of all let us go back to our simple solution  $t_{1/2}$ , because we are we have the value of  $t_{1/2}$  given here, that is what is it 5745 years. So,

$$t_{\frac{1}{2}} = \frac{0.693}{\lambda}$$

So, we can find the value of lambda from here

$$\lambda = \frac{0.693}{574.5 \times 365 \times 24 \times 60 \times 60} = 3.83 \times 10^{-12} \text{ s}^{-1}$$

The value comes out to be something like  $3.83 \times 10^{-12}$ , you can check my calculations again I have done it very quickly.

Now, our next task is to find out the weight of barium carbonate. We know one thing, that is the number of atoms that are decaying proportional to the total number of atoms that are present. So, number of atoms decaying proportional to total number of atoms present which basically means that what do we have here? We have a simple first order reaction.

So, now, what we can do? We can use the simple expression for first order reactions and that would be

$$-\frac{dN}{dt} = \lambda N$$

And now, the  $\lambda N$  can be expressed in terms of weight and molecular weight. So, we have let us say weight is  $W$ . So, we need to calculate this and that will be divided by the molecular weight of barium carbonate. And if we need to find the number of atoms, what do we need? We need one more something else which is the Avogadro's constant. So,

$$-\frac{dN}{dt} = \frac{\lambda W}{199} \cdot 6.023 \times 10^{23}$$

This again this gives me a value  $1.16 \times 10^{10}$  W! we do not really now know the value of  $W$ .

(Refer Slide Time: 03:53)



$$\begin{aligned} \# \text{ atoms decaying} &\propto \# \text{ atoms present} \\ -\frac{dN}{dt} &= \lambda N = \lambda \frac{W}{199} \cdot 6.023 \times 10^{23} \\ &\approx 1.16 \times 10^{10} \cdot W \text{ s}^{-1} \\ 1 \text{ mCi} &= 3.70 \times 10^7 \text{ d/s} = \frac{-dN}{dt} \\ W &= \frac{3.70 \times 10^7}{1.16 \times 10^{10}} \approx \boxed{3.19 \times 10^{-3} \text{ g}} \end{aligned}$$

However, what do we know here? We know that the activity that we need to get is 1 mCi. Now, interestingly what is 1 mCi? This actually equals  $3.70 \times 10^7$  decays per second. So, 1 Ci equals  $3.70 \times 10^{10}$  decays per second. So, remember since we are talking in terms of decays. So,

$$1 \text{ mCi} = -\frac{dN}{dt}$$

From here we can now find the value of W. So, W will be equal to what?

$$W = \frac{3.70 \times 10^7}{1.16 \times 10^{10}} = 3.19 \times 10^{-3} \text{ g}$$

So, this is your final answer.

(Refer Slide Time: 05:07)



$$\begin{aligned} \underline{G \text{ to } D} \quad \Delta G_{rxn} &= \Delta G_D - \Delta G_G \\ &= 2.9 \text{ kJ/mol} \\ k &= e^{-\Delta G/RT} \\ &= e^{\left(\frac{-2.9 \times 10^3}{8.314 \times 273}\right)} \\ &= 0.278 \\ \Delta G > 0 \quad ; \quad k < 1 \quad \text{Not feasible.} \end{aligned}$$

Another very simple problem; the problem of conversion of graphite into diamond. So, you already know that graphite to diamond is not really feasible. You already know that graphite is the most stable format it has the 0 formation of energy. That is already clear from the problem statement but let us see how we can calculate the reaction constant and that will also tell us that this is not feasible reaction.

So, we have here  $\Delta G$  of reaction; this is what we need to calculate that would be

$$\Delta G_{rxn} = \Delta G_D - \Delta G_G$$

So, these values are already given, you will see that this is +2.9 kJ/mol, because for graphite it is 0 anyway. And then, how do you calculate the reaction constant k?

$$k = e^{-(\Delta G/RT)}$$

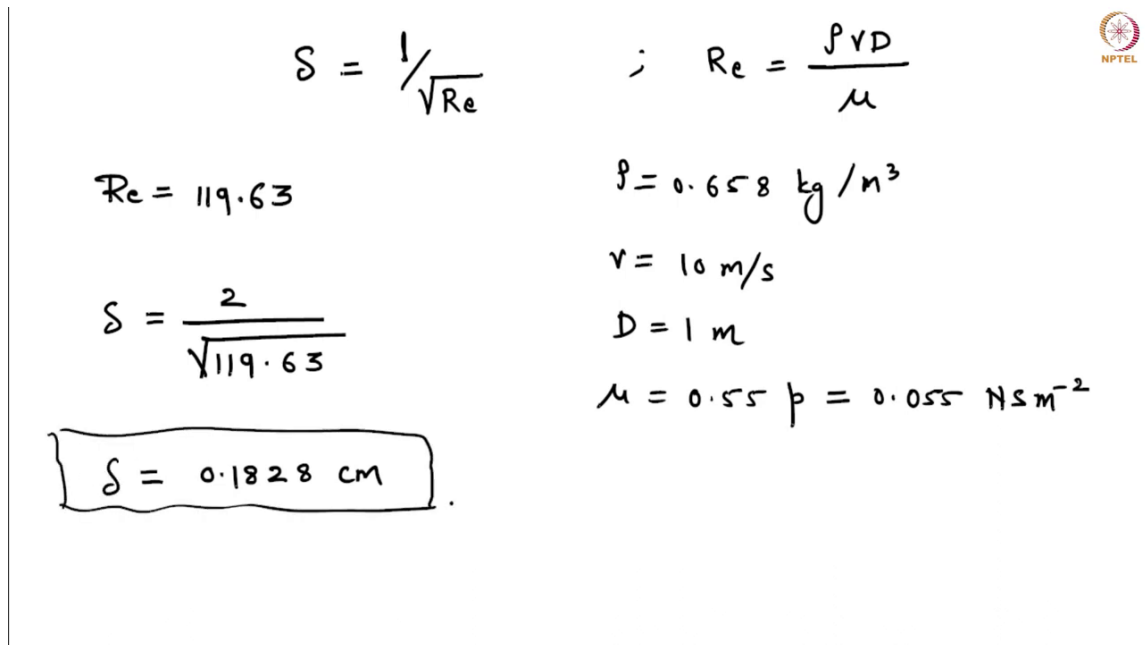
So, just keep in mind the units and you should be fine this is a very simple problem.


$$k = e^{\frac{-2.9 \times 10^3}{8.314 \times 273}}$$

This will give you a value which is approximately 0.278. So, this is basically the solution of the problem, you just need to see that the  $\Delta G$  of this reaction is greater than 0.

So, it is the positive value and now you also see that the value of reaction constant is smaller than  $k$  so, both conditions suggest that this is not a feasible reaction at standard room temperature and pressure. So, we are done here.

(Refer Slide Time: 07:03)





$$\delta = \frac{l}{\sqrt{Re}} \quad ; \quad Re = \frac{\rho v D}{\mu}$$

$$Re = 119.63 \quad \rho = 0.658 \text{ kg/m}^3$$

$$\delta = \frac{2}{\sqrt{119.63}} \quad v = 10 \text{ m/s}$$

$$\quad \quad \quad D = 1 \text{ m}$$

$$\quad \quad \quad \mu = 0.55 \text{ p} = 0.055 \text{ Nsm}^{-2}$$

$$\boxed{\delta = 0.1828 \text{ cm}}$$

So, this is the numerical problem on the CVD reactor, what do we need to calculate here? We need to calculate the boundary layer thickness which is

$$\delta = \frac{l}{\sqrt{Re}}$$

So, first we need to calculate the Reynolds number, which is

$$Re = \frac{\rho v D}{\mu}$$


So, all these values are given to us.  $\rho = 0.658 \text{ kg/m}^3$ ,  $v = 10 \text{ m/s}$ ,  $D = 1 \text{ m}$  and  $\mu$  or viscosity is given to us as 0.55 pois which equals  $0.055 \text{ Nsm}^{-2}$ . So, now, from here I have calculated the value of Reynolds number as 119.63, you can also calculate it for yourself.

And once we have the value of Reynolds number now, boundary layer thickness is very easy  $l$  is given in centimeter. I can just leave it in centimeter because it does not matter Reynolds number is a dimension less number. So, if I take it, if I take my  $l$  value in

centimeter then I am going to get also the boundary layer thickness in centimeter. So, from here what I get is 0.1828 centimeter. So, that is basically my final answer.

(Refer Slide Time: 08:37)

$$\begin{aligned}
 &\checkmark \text{ Energy} = 200 \text{ mJ/cm}^2 \\
 &\text{Lamp intensity} = 8.2 \text{ mW/cm}^2 \\
 &\frac{200}{8.2} \approx 24.39 \text{ s} \\
 &\qquad \qquad \qquad \approx \underline{\underline{25 \text{ s}}} \\
 &\underline{\text{SiO}_2} \quad \text{glass} \quad \underline{1.5 \times}
 \end{aligned}$$

Resist datasheets   
 20 - 40  $\mu\text{m}$  :  
 200 mJ/cm<sup>2</sup>  
 150 —

So, this one is a very simple problem really. So, you are given the energy that is required for cross linking the film of your resist. And you are given the intensity of your lamp. Now in general what happens is, you do not really know the energy in the beginning whenever you are using a certain type of photo resist. Then these resists will come with what is known as the data sheets. Especially, when we are talking about the negative photo resist.

Then, we often have data sheets that are provided by the vendor and in that data sheet you will often have this information for which thickness, what is the energy that is required. For example, for 20 to 40  $\mu\text{m}$  for any given resists, they may be let us say 200 mJ. And it can be so; for 50  $\mu\text{m}$  it can be a different and for 150  $\mu\text{m}$  it will be different; for 5  $\mu\text{m}$  different. So, you have to first learn how to read the data sheets which is not very difficult.

From the data sheets, you can figure out what is the energy required. So, here I have already given you the value of the energy for cross linking and now your lamp intensity is also given; but again in the clean room what you may have to do is there are intensity meters which you need to use to get the value of the intensity at that given point, because

often when you buy, for example a mercury lamp for UV exposure; over time their intensity decreases.

So, at any given point what is the intensity; the best option is to measure it on that day just before your experiment. If these are the 2 values and you need to calculate what is the exposure time well, since everything is given nicely in the same type of unit;  $\text{cm}^2$  and also mJ, mW. All you need to do is you just need to divide your energy by the intensity of your lamp that is all. So, basically this comes out to be something like 24.39 seconds.

Since you cannot expose for 24.39, you will expose it for 25 seconds. Now, here a few more important things which I have not mentioned in the question, but I should tell you. I told you that this experiment is been performed on silicon wafer.

I have written that for a reason, because if you do not have silicon substrate and you have silicon oxide substrate or let us say you are not making this entire structure on silicon at all and you are making it on a glass or quartz substrate. Or there can be other substrates; sapphire substrate, you can choose different, even ceramic substrates for certain applications. In that case, you need to also see if your resist requires the same kind of energy or different; you have to factor something else in.

For example, often in the case of glass, you require 1.5 times the energy that you require for silicon wafer. So, these kinds of things are also mentioned in the in your data sheets. So, you definitely need to check for all these things before you calculate your exposure time.



(Refer Slide Time: 12:06)

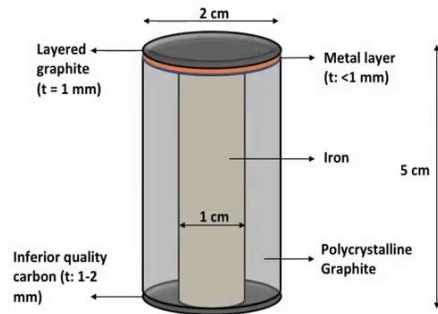
स्वाति शर्मा, भारतीय प्रौद्योगिकी संस्थान मण्डी

### Problem Set



**Mention all the steps, materials, methods and parameters to manufacture the following:**

A hollow polycrystalline graphite cylinder that contains cast iron filling as shown in Figure below. The top plate has a layered graphite structure with a mosaic spread of  $0.8^\circ$ . Between the top graphite plate and the cylindrical structure, there is a thin metal layer (any metal can be chosen). The carbon in the bottom layer should be of lower purity and contain porosity. Note that after filling, iron should not be heated  $>900^\circ\text{C}$ . There should be no glue/ adhesive or weak joints.

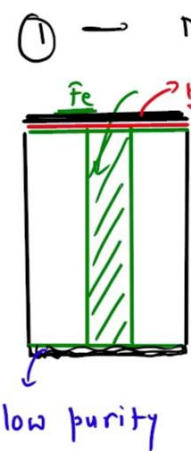


Now, we come to a manufacturing related problem. So, you can see in this problem, I have given you a certain shape or certain cylinder of graphite and you have to fill some iron inside it and then there are some other parameters that you can see in this problem. Now, the thing is, this is one structure and it contains three different types of carbons. So, you have graphite cylinder and then you have HOPG and then you also have some low purity carbon and then of course, some other metals.

So, how would you go about making such a structure? Let us solve it. So, how do we go about making this kind of cylinder? So, first of all we need this hollow cylinder and inside that we need iron filling. So, the first thing that comes to your mind is we can perform casting for filling the iron.

You can also insert an iron rod and either way what you would need is first you would need your hollow graphite cylinder. Now, I said casting because graphite itself can serve as a refractory material. What does that mean? It does not lose its any properties or its mechanical strength at high temperatures even at very high temperatures.

(Refer Slide Time: 13:29)



① — Manufacture graphite cylinder  
Needle coke + pitch/resin →  $>2600^{\circ}\text{C}$

② Casting of Fe

③ a)  $0^{\circ}\text{C}$  — HOPG  
Pyrolysis of HC  
Top-layer  
Cu layer / Ni layer

④ Any polymer: charring  
 $\Delta 900^{\circ}\text{C}$

⑤ b) Hot-pressing —  $2600^{\circ}\text{C}$

low purity

We can have a hollow cylinder made of graphite. So, that is going to be our first step. We manufacture the graphite's cylinder itself. And how are you going to do that? Well, you have learned a few techniques for that and also you know the precursors. For example, you can make it using needle coke or you can make it also using some other polymer for example, PVC. And the most common one would be needle coke and either a pitch or resin binder.

And then, basically, you will heat treat it. This you can see in the needle coke lecture. So, you will first heat treat it at lower temperatures say  $1000^{\circ}\text{C}$  and then you will have to perform the pore filling operations. And finally, you have to go to very high temperatures, let us say  $26000^{\circ}\text{C}$  for getting the graphitization.

Now, what you have? You have your cylinder ready. So, this is your hollow cylinder. So, this is the structure that you have now made. I can also cover it here; this is your front view of a cylinder. What is next? Now, you need to fill the iron inside your; this is where you need to now have your iron filled. So, what can you do? The second step can be casting of iron.

You can perform the casting and you now have your cylinder also filled with iron. Now, what is the next step? The next step you need to do is now, you need to make the top layer. If you remember the top player needs to be graphite layer again. However, there

should be some metal layer in between and we can choose any metal for that purpose. So, let us say here I need a metal layer. So, what do I do now? The top part looks like HOPG because we have 0.8 degree of mosaic spread and this is the HOPG part and for making HOPG, the standard process is basically pyrolysis of a hydrocarbon you can also call it a CVD. Basically, this is the pyrolysis of hydrocarbon. So, this is our step number 3. So, this is for making the top layer.

Now, remember that before we perform the pyrolysis of hydrocarbon, what you anyway require is a catalytic layer. So, this is similar to what you have for graphene CVD. So, you have a copper layer or you can also have a nickel layer depending upon what thickness do you need. So, typically we would take nickel layer because copper layer tends to have only a few layers of carbon deposited.

Now, we take the nickel layer and then on top of that you pyrolyze your hydrocarbon. One important thing is that, when you want to convert these hydrocarbon layers into graphite, you cannot really anneal out the entire structure at very high temperatures, because in the question it is mentioned that your iron should not be heated above 900 °C. So, what else I can do? I can perform hot pressing.

So, rather than annealing out the entire structure. So, let me call this 3a and this is my 3b step. There I will perform heat hot pressing and then I will go above say 2600 °C, very similar to the graphitization temperatures. So, then I get my top layer.

Now, all we are left with is the bottom carbon layer. And bottom carbon layer can basically be porous and low quality that is what is mentioned in the question. So, what does this mean? Well, porous low-quality carbon; we can basically make at temperatures as low as 900 °C. So, that is we do not destroy, or we do not harm the iron because it should not go above 900 °C.

If we need intentionally the porosity, then in that case, we will take any polymer which goes through charring process. However, if your question says that well porosity is acceptable in that case you can take any polymer, but since we have specifically mentioned that there should be some porosity in the structure, then we will take some polymer that undergoes charring, for example, some cellulose or something.

And then heat treat it at 900 °C and then what we get is some low quality. So, basically low purity carbon with some porosity. So, this is your low purity carbon which we can get at 900 °C. So, that is basically that is your entire structure.

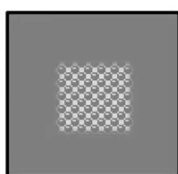
(Refer Slide Time: 19:02)

स्वाति शर्मा, भारतीय प्रौद्योगिकी संस्थान मण्डी

#### Problem Set



1. A solid cube made of a resin needs to be converted into carbon at 1200 °C. Final (carbon) structure may have its edge length anywhere between 1 mm and 1 cm. If the cube is too big, it might contain some porosity in its core (as shown in the cross-section of the cube, see Figure below). Dimensional shrinkage of this resin is ~50%, but nothing is known about its pyrolysis mechanism and by-products. **Design a single heat-treatment experiment to determine the maximum size of the cube that can be made without any porosity.** You will have sufficient supply of resin and any other material(s)/ manufacturing process, if needed. After the heat-treatment, you are allowed to use up to two characterization techniques of any kind.
2. For a polymer of unknown chemical structure/ properties, how would you experimentally determine whether it goes through coking or charring?



Cross-section of a carbonized cube containing pores in its core.



Yet another problem related to making carbon structures but here we will be talking about how to make structures from polymer to carbon. Basically, how do we optimize, how do we come up with the exact dimensions of our precursor material. So, I have not gone into the details of how much shrinkage your polymer has, because in this problem you can already see, the shrinkage parameters are not provided to us.

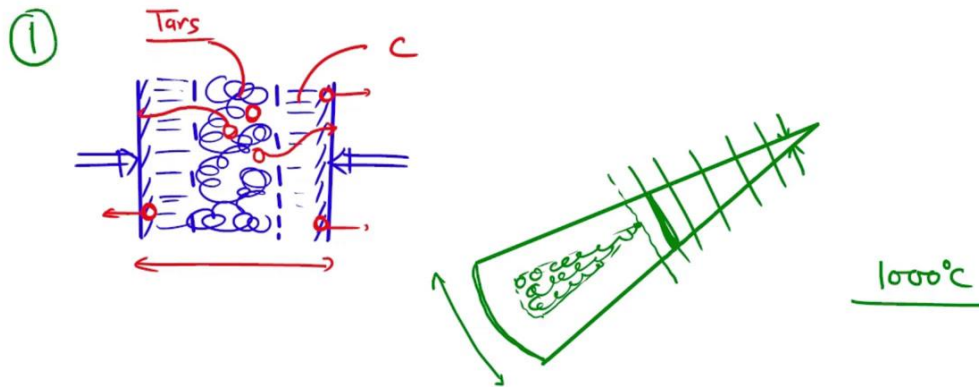
What we just need to find out, at what dimension do we get porosity-free structure? So, I think this problem I had also mentioned in one of the lectures but now when it comes to manufacturing maybe you will understand a little more details when we solve it again.

This problem looks more complicated than it is actually. I have written a lot of story in the question statement. Basically, the question is, if you do not know anything about a polymer you just go to the market and you purchase a certain polymer or let us say you buy new equipment which comes with its own polymer.

So, for any given reason, if you do not know anything about the polymer, then what can you guess about these structures? And say you can only fabricate at 900-1000°C or

whatever given temperature. And you have certain capabilities of the equipment of your furnace and then you need to find out whether or not I will get porosity-free carbon. So, whenever we make any structure.

(Refer Slide Time: 20:34)



Let us say when I have this structure now; let us say some parts, which are closer to the surroundings. They get heated up and they start to become carbon, they start to get carbonized and this process continues.

But you should also know that the material; which is in the middle, this material is still not completely carbonized yet and it has a lot of bubbles strapped inside and because there are a lot of gases being produced and those bubbles will need to get out and they are still far from the surface.

So, they find it difficult to anneal out; however, the bubbles that will be forming here near the surface will anneal out quickly. That is basically your problem. There will also be some thermal conductivity difference because this material is already carbon.

Let us say, at a given temperature while this material still contains a lot of tars and bubbles. Of course, there is going to be also thermal conductivity difference. So, the temperature which is reaching the core of this structure may not be the same as what you

have on the surface. So, due to all of these things, the core remains let us say uncooked while the surface gets cooked. So, this is the problem.

What do you do? If you are given any polymers, so whatever I have asked in the question, what you can actually make is something very simple. You can make a wedge like structure, like a piece of cake. Sy this is your structure. So, this is your wedge; this is the top view of your wedge and.

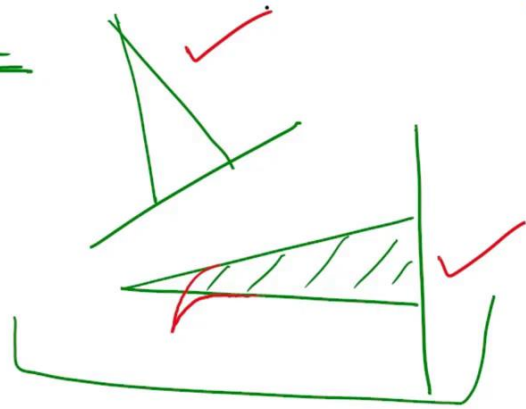
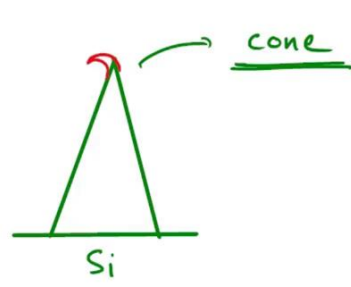
Now, you just heat it inside the furnace. I said that you should design one experiment, whatever is the temperature you want to use. Let us say 1000 °C. So, now, you place your piece of cake inside that 1000 °C furnace and what you will now get is some part that still contains porosity.

You can see because of this wedge-like structure, the thickness or the end of this wedge is much smaller compared to what you have over here. Basically, due to this gradual decrease and after you remove it from the furnace, then make a lot of very thin slices and there will be a certain point where you will be able to see some porosity.

So, basically whatever is the length at this point is the maximum dimension you can get. So, this is basically a rather simple problem. Now, coming to the second problem. So, this was the first one and the second problem that is also very similar basically I have just asked you.

(Refer Slide Time: 23:50)

2



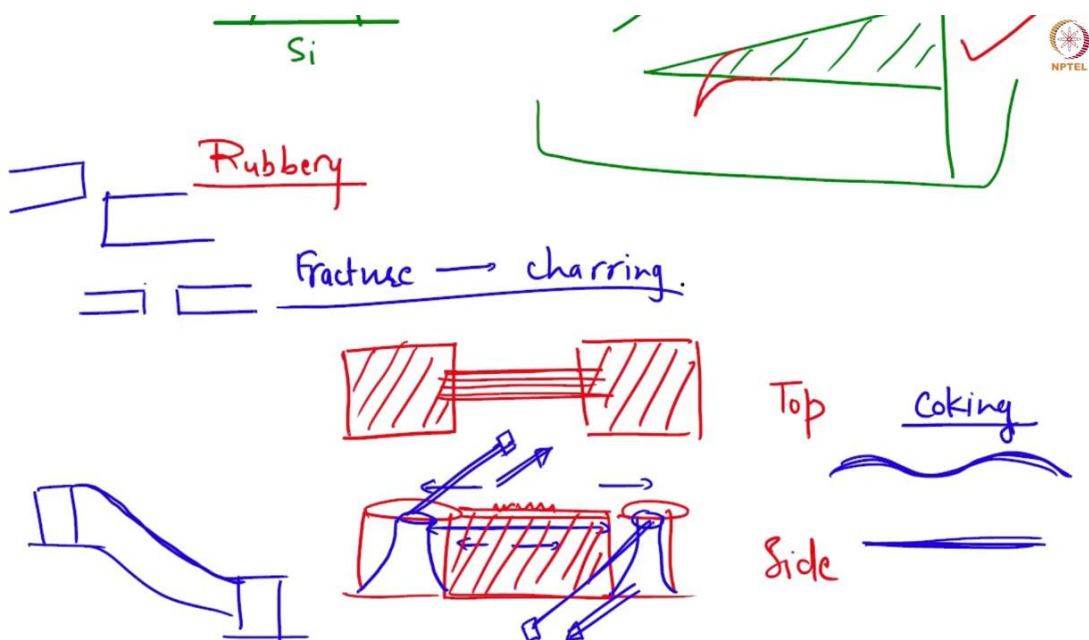
Rubbery

How do you know if your polymer is going through coking or charring? So, coking and charring; this is something that you have to often experimentally figure out especially if you do not know anything about the polymer. So, what you can do is you can make structures that can potentially bend.

I think I had also shown you some figures, which look like this; so this is a cone. You can make these cone-like structures using your polymer, and then let us say this is my silicon substrate. Now, when I place it in the furnace, I can place it like this or I can place it also like this. This is being my sample holder. So, I can place my structures in different ways, if this structure does undergo coking, in that case after the pyrolysis, you will find some sort of bending.

Or even if the polymer goes through too much of a liquid state, not a semi-solid; but rather a viscous liquid type state, in that case, even when your tip is standing up you will find some sort of bending. But if that is not the case because in most cases, many polymers just go through a rubbery state, or semi-solid whatever you want to call it rubbery state not a liquid-like state. So, in that case, you will need to perform; you know you will need to place your sample in such a way, that you can observe some sort of deformation afterward.

(Refer Slide Time: 25:34)





You can also make structures where for example, I make you know two pillars of polymer. And then on top of these pillars, I place another say, either a thick fiber or some other structure; all of it let us say so it is a ribbon-like or a thick fiber-like structure. Now, this is the top view. So, this will be the side view, you have 2 pillars something connecting them. This is the side view this is top view.

So, in that case, what will happen after your pyrolysis because your pillars are also shrinking? Then they will have some deformation; either this structure, this fiber or ribbon or strip whatever you had this will get elongated. So, this is also one more thing that you can do.

Instead of this fiber, you could also have made an entire wall; it depends of course on your fabrication capabilities, but if you make a wall between these two pillars; in that case, your wall may also be deformed afterward. You can also make structures which are being pulled. So, let us say this pillar is connected to another pillar here and this pillar, in another direction is connected to something.

So, basically during the pyrolytic shrinkage, this pillar will be pulled in this direction, the other one will be pulled in this direction; in that case, your wall will be twisted, you will get something like this when you get the top view. After pyrolysis and then you have your pillars.

Basically, these are the kind of structures; the idea is to make non-uniform stresses or structures with which will after shrinking undergo non-uniform stresses and then you can accordingly study the deformation behavior. If you do see deformation, but a continuous structure. So, your polymer let us say your wall became like this, but it did not break or your whatever was the fiber it got pulled, but it did not break it just became thinner. In that case, this is your coking process. If you have a polymer which rather than twisting or bending it breaks. So, if you had a charring kind of mechanism, then let us say whatever was your fiber that breaks or if you had the wall, it does not really show bending, but you know two separate structures like that.

So, if there is any kind of fracture in the structure, in that case, you can say that this is your charring process. Basically, these are some of the simple experiments that you can perform.

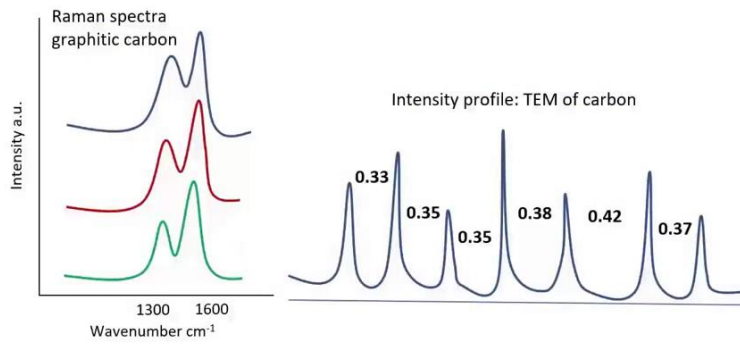
(Refer Slide Time: 28:34)

स्वाति शर्मा, भारतीय प्रौद्योगिकी संस्थान मण्डी

### Problem Set



1. Determine the increase in graphitic content, if any, from the set of Raman spectra shown in Figure 1. These values are for a disordered carbon material heat treated at various temperatures.
2. In Figure 2, intensity profiles of a disordered carbon material, as observed in a transmission electron micrograph, are shown. Comment on the stacking of sheets and the nature of carbon. Is this a top or a side view of the stacks in your opinion?



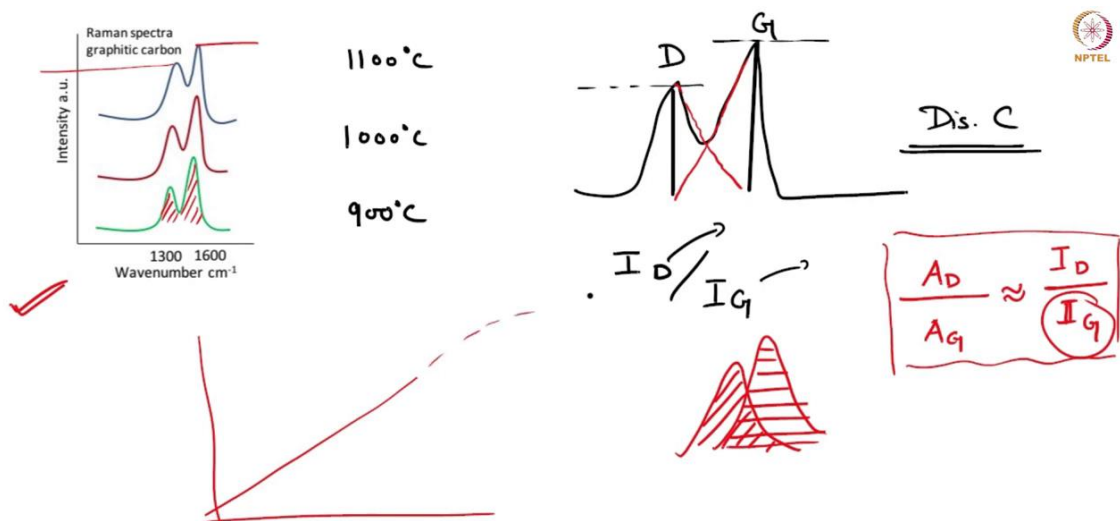
Finally, we solve a couple of problems related to the characterization techniques; again X ray diffraction we had already solved one problem when we were discussing the lecture. And now also I do not remember, but maybe I did tell you few things about the Raman spectroscopy.

And also definitely we discussed when it comes to TEM images; how to correctly interpret them, but these problems will probably also help you because these are more related to the practical problems that you will face during making something using carbons.

For example, the first one is on Raman spectroscopy. Raman spectroscopy is used at different temperature points; as you increase the graphitic content for example, graphitic carbon can be graphitizing or non-graphitizing type.

When we say graphitic; now you know the definition of graphitic anyway. So, here using the Raman spectra of the same carbon material at 3 different time points or temperature points, how do we determine if there is any increase in the graphitic content? So, that is your Raman spectroscopy problem and the TEM problem is very simple, you have an intensity profile and what kind of staking do you have in your carbon material.

(Refer Slide Time: 29:51)



I have again pasted all the Raman spectra here. So, this is some carbon material, let us say, it is some sort of disordered carbon material, we get it from polymer and we keep on heating it say at 900 °C and then at 1000 °C and let us say this one is at 11000 °C. So, we need to find out what is the optimum temperature or if there is an increase in the graphitization or the graphitic content in our carbon material.

We can do that using Raman spectrum. So, we know that disordered carbon materials will have this kind of Raman spectrum and they will have 2 bands D and G band. So, we are not talking about graphite. as you can see in this spectrum itself, this is that of a disordered carbon material. now, one standard method for finding out what is the change in the graphitic content is to divide the intensity ratios intensity of these peaks.

So, ID/IG or you can also do it the other way around IG/ID, but you should know that when you write D then this is for the D peak and G is for the G peak. Often people would measure just intensity; intensity means just this height in both cases.

So, that is your intensity, but in principle because your peaks are merged. So, what you have here is not really too clear peaks because your D peak can also be like this. So, we also saw this in the class and then your G peak can also be like this.

So, you will have 2 different peaks and what you need to do is, if you want to get more accurate information; in that case, you need to fit these peaks and you need to find what is the actual area of individual peaks. So, rather than intensity or rather than just the high of the peak, what you would rather calculate is the area of both peaks. Basically it is your area of the D peak divided by area of the G peak, but we still consider it or call it at least ID/IG ratio.

And this ID/IG ratio will keep on either increasing or decreasing and depending upon that you can figure out what is your increase in graphitization. in this case, here I am not really able to calculate the area of each peak, because you will need to find the best fit. So, you might indeed have 2 or 3 different types of values and you need to find the best fit value and in that case, this formula you can find.

If if the intensity of your G peak intensity or area is increasing. So, the ratio might be decreasing if you are taking ID/IG. And so in that case, either you can calculate it using the intensities the heights of the peaks or the area of the peak.

And then you can find out your ID/IG ratio typically within a certain range. the ID/IG ratio will have a linear increase and that linear increase will tell you whether or not, you have more graphitic or more disordered content. However, if the disorder increases too much; in that case, you may not get a linear increase. So, remember that, but for most practical purposes this method is very useful and this is how you calculate it.

So, again I have pasted the same intensity profiles. What do you see here? You see that there is some value 0.33, 0.35, 0.35. So, the first three values actually look like they might be the values for some sort of graphitic carbons. You know that for perfect graphite you have 0.335 nm and solve these values are in nm. But you will get values up to 0.36 or even slightly higher. Even then it is acceptable in the case of disordered carbons.

Now, why I am saying, if you remember at some point I told you that 3.44 Å or 0.344 nm is the limiting value for turbostratic carbon. First of all, that value has also been debated to some extent and it is acceptable that up to 0.36 nanometer.

You can still call it disordered or you can call it turbostratic carbon. However, there is also one additional factor when we are doing these manual calculations of the distance between the 2 intensity peaks; in that case, there is some manual error or there is a possibility of manual error.

So, in that case, let us say up to 0.36 nm; we just call it acceptable in your graphitic carbon or at least graphitic turbostratic carbons. So, when I say graphitic that means, that this is an annealed carbon. So, graphitic turbostratic basically annealed at high temperatures; this might be glass-like or activated carbon sample. Now, the first three values are acceptable, but after that you have 0.38, 0.42 and 0.38.

Now, these values do not look like the values of even an annealed carbon. What does that mean? Of course, this intensity profile was taken on your annealed carbon sample. So, that basically indicates that, it is not that this is another material or impurity or something like that; what it indicates is that you are not looking at the side view of your stack. So, let us say if I had my stack like this. For the first three values for say it is 0.33, 0.35 and 0.35.

So, in that case, I would assume that I am looking at the cross-section. So, when I say the first three values then I am looking from here. But, when we see the other three values it is quite possible that we are looking at some sort of top view. So, it could be something like this and now we are looking from the top. So, this is also possible and that is the reason for the values that you are getting.

Let us say what you are getting this distance here, maybe this can be 0.4; it can potentially be anything. So, this is one possibility; another possibility is that what you have here is, after three layers what you have is probably a lot of defects.

And because of the defects you have more spacing between the layers, it can also be some other layers coming from a distance and then these values here. Then these values are some random values, but in some region, you can say that there is a little bit of graphitic content in your carbon material.