Chemical Engineering Principle of C V D Processes Professor R. Nagrajan Department of Chemical Engineering Indian Institute of Technology Madras Lecture No 02 CVD Reactor and Process Design Fundamentals

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Good morning. Welcome back to this course on chemical engineering principles of C V D process. In the last lecture, we introduced some basic principles of chemical vapor deposition and to reiterate the key point from the last lecture, in chemical vapor deposition the identity and the composition of the condensate that forms is different from the identities and composition of the species in the vapor phase that lead to the formation of that condensate. So for the formation of the single condensate species like silicon a variety of gas phase reactants could participate in the deposition process. They can react among themselves and the transport process from the bulk of the vapor phase to

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the substrate will take place through the diffusion of many, many chemical species that contain the depositing element.

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Now the advantage, the primary advantage of C V D over physical vapor deposition where the identity of the condensate exactly matches the identity of the vapor species is that it is much more energy efficient because you are essentially taking advantage of the natural tendency of gases in a high temperature system to dissociate and form a variety of species. And also as species dissociate and they become lighter the diffusion rate increases. Because the diffusion rate of the particle as well as species is inversely dependent on its size.

So the smaller the molecules, the faster they will diffuse. So the fact that in chemical vapor deposition you have extensive dissociation of the gas phase molecules into smaller precursors also results in an enhanced rate of transport of these precursors to the substrate. In addition to the advantages that we talked about last time that C V D essentially results in very uniform coverage over a surface. It is able to follow contours much better than other types of deposition processes and the purity of the system can be maintained quite effectively.

As chemical engineers we are always concerned with the design of a system. How do you design a C V D reactor? What are the key components in it? What are the factors you have to take into account when you design a C V D reactor? So let us take a look at that a little bit. So a C V D reactor is in essence no different from any chemical reactor, which means that you have reactants flowing into the reactor. You provide some source of energy to make the reactants come together, reactants form a product and then you have a mechanism by which the product can be removed and any byproducts can be exhausted from the system. And just like with any chemical reactor, you have to provide appropriate controls to make sure that the reactor performs in a very consistent and repeatable and reproducible manner.

So if you look at a C V D reactor in its most basic configuration,

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you have gases essentially entering

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on one side of the reactor and flowing through the reactor and exiting at the other side of the reactor. There is a substrate holder or what is known as a susceptor which is fixed typically to the bottom of the reactor. It is on top of the susceptor that deposition must take place.

So the deposit will actually form on top of this receptor or susceptor that is introduced essentially to make the condensate form.

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Now the reason that condensation will happen here and not here or here is what,

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do you have a feel for why condensation will form, will happen only at the interface between the surface and the gases? What is the difference between the rest of the reactor and the interface?

(Professor – student conversation starts)

Student: Temperature of the interface should be lower compared to...

Professor: No, actually there are 2 configurations. There is something called the hot wall reactor and the cold wall reactor. And by the way, in C V D systems, the higher the temperature the greater the chance of deposition. So actually condensate will be maintained if anything at a temperature that is hotter than the surroundings in order for the deposition to happen. That is not the primary reason. Even if you have a uniform temperature distribution in the reactor, deposition is more likely to happen on the substrate rather than in the gas phase, why is that?

Student: The other reactant is present 0:05:40.0 on the substrate.

Professor: Yes?

Student: The other reactant is...

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Professor: No, all the reactants are introduced here. So the reactants are introduced on the left side of the reactor and the products and the byproducts are being taken out and the condensate is forming

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here. So that is not the reason Student: The solids...

Professor: Impact is only an important phenomenon when you have large particle sizes, you know. Fine particles and vapor molecules do not impact. They just diffuse and they either stick or bounce off, so...

(Professor – student conversation ends)

Ok the primary difference is that this is a heterogeneous process versus a homogenous process. When you look at how a C V D film is formed you do not immediately form a continuous film. You initially nucleate droplets of the condensate. So it is essentially a nucleation process. And the energy barrier for heterogeneous nucleation is much smaller than energy barrier for homogenous nucleation.

So thermodynamically, there is a natural tendency for chemical vapor deposition to happen on any surface that you introduce regardless of what temperature you keep it at, what surface energy it has and all that. So that helps. Because in a C V D reactor, you do not want homogenous nucleation to happen. You do not want little silicon particles forming, you know, here, here, here, and then trying to deposit on the substrate.

That would not

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be good because what will result is a very flaky, powdery deposit rather than a continuous and well-adhered film. So the entire point of the C V D reactor is to design it such that the formation of the condensed phase only occurs at the substrate on which deposition is supposed to happen

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and you completely suppress its formation anywhere else in the reactor.

Now in essence that is actually very different from what is known as chemical vapor synthesis reactor. In a C V D reactor, you want the condensation to only happen here.

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In what is known as a C V S reactor or a chemical vapor synthesis reactor, you actually use the reactor to make nanoparticles and the way you do that is by promoting homogenous nucleation and getting these very, very fine particles to form in the gas phase and then providing a mechanism for them to agglomerate and form larger particles which can grow to their nanometer size and then you suppress it. You essentially freeze it at that point.

But, anyway that is good when you are trying nanoparticles but when you are trying to make a C V D film, you want the exact opposite to happen. You want to design it so that thermodynamically and kinetically, it is very difficult for any particles to form in a gas phase and virtually all of the condensation only occurs at the substrate that you have introduced into the reactor.

Ok so if you look at this very basic configuration, you can see that what you are relying upon is that once you have this reactor, you bring the reactants in. You bring it up to whatever temperature and pressure that you want to run it at. The reactions happen and the condensation happens here. And essentially all the byproducts are then exhausted out. The substrate is removed and the film is then inspected and, and used for further processing, right?

Now what are some of the drawbacks in this design? Let us say that you are using, as we said last time, silane and pyrolyisis process to make silicon, Ok. So the silane is introduced in this direction

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and the temperature is designed such that it starts to form various precursors of silicon and you start condensing silicon on the substrate. Do you think you will get a uniform substrate? I mean uniform film on the substrate, or will the thickness change as a function of downstream distance?

(Professor – student conversation starts)

Student: Thickness will vary as a constant gradient of the reactants

Professor: Yeah basically what will happen is that the, the concentration of silane here will be quite large when it first encounters the substrate.

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But some of it will then deposit. So the precursor concentration itself will start decreasing, right? If the gases are flown across the substrate. And therefore what you would see is that

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you will get a very thick deposit, the leading edge but as you go towards the trailing edge of the substrate you will start seeing a reduction in the thickness of the deposit which is not good. So how do you address that situation?

If you are a chemical engineer and you are trying to design this process and you want to get uniform film, how would you do it?

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Student: Increase the velocity?

Professor: Increasing the velocity may reduce the severity of the problem but you will still get a non-uniform substrate.

Student: Inclining

Professor: Yeah, inclining the substrate is one way to do it and that is one of the tricks that, that is used in the industry to try and get a more uniform deposition; any other ideas?

Student: Rotate the substrate

Professor: Rotating the substrate can help, yeah.

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But you still have this basic problem that there is a depletion of the reactant concentration as it flows across the reactor. Ideally what you would like to see is that the reactor, reactant concentration is maintained

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uniform across the reactor, you know, wherever the substrate is. (Professor – student conversation ends)

So, the way to do that is to introduce a carrier gas. So instead of just flowing silane through the reactor, you will essentially take a silane with, for example H 2 mixture and in fact the silane concentration will be kept around 10 to 20 percent and the H 2 concentration will be kept at 80 percent so the hydrogen gas in this case is used as a diluant. It lowers the concentration.

Now when you do that what happens? The concentration, the silicon or the silane concentration can be maintained virtually constant as the gas flows across the substrate. So use of a diluting agent helps in maintaining uniformity of the film thickness. Any other ways you can think of?

Suppose you don't have to flow the reactants left to right, you know, in other words parallel to the substrate, suppose you could flow it vertical, would that help? So for example, if instead of this type of flow configuration, supposing you were to do, introduce the gas this way and essentially achieve a stagnation point flow,

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would that be preferable?

(Professor – student conversation starts)

Student: The sides, there may be the formation of the...

Professor: Ok, the formation of deposits on the sides; that is not a big issue, you know, that is not a critical functional

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area of your substrate. And again I think that can be minimized. But as far as the front, the deposition surface, will you get a more uniform substrate with vertical stagnation flow? You do.

(Professor – student conversation ends)

In fact, because essentially when you do it this way, the entire layer here, I mean, obviously you have to design it so that the stagnation flow happens with the entirety of the deposition surface being in the stagnation zone but if you can make that happen then you are liable to get a more uniform substrate. But are there any drawbacks to that setup? What could be a problem with this type of flow?

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Or let me ask you this way?

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When would you use this flow versus this flow?

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The, one of the

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characteristics of the vertical flow is that the residence time of the vapor in the vicinity of the substrate basically becomes infinity because there is no way for it to, no place for it to go. So what does it mean? Over time you are going to grow very, very thick deposit, right? Whereas with the horizontal parallel flow, you can achieve a much thinner film

So essentially the vertical stagnation flow is typically used when you need C V D films that are of the order of many nanometers or even microns thick where as if you are trying to make a very, very thin and uniform C V D film, then you prefer to use the parallel flow. So if you look at the components of a CVD reactor, what are the critical components? So you need good gas delivery system. All the reactant gases

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have to be delivered to the reactor in such a way that they do not react on the way. So either you have to have multiple inlets for the reactive gases or you have to ensure that the temperature and the pressure conditions during the flow into the reactor or such that chemical reactions cannot happen that result in the formation of the condensate.

The second part of it would be the chamber itself. And

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again the design of the chamber would depend very much on what mode you are going to use. We will discuss later that you can have high temperature reactors, lower temperature reactor, atmospheric pressure reactors, low pressure reactors, so depending on the operating conditions that you choose, you will have to appropriately design the reactor.

The third part of it is the substrate on which you are going to

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OMPONENTS

condense the C V D film, and related to that is the loading mechanism, loading slash unloading mechanism

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and the substrate has to be provided a separate source of energy. The reactor itself may have its own energy source so that you can maintain the entire reactor at a certain temperature and so on. But in C V D systems, typically the substrate will be maintained at a temperature that is different from the reactor itself.

So you need an energy source, some kind of typically a heater if you are going to provide thermal energy and by the way there are different ways in which you can, you can provide the thermal energy to the system. You can

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have radiative energy sources, you can have r f sources, you know, so you can do tube furnace type of arrangements. Or you can use an induction heater and so on. So providing thermal energy is one way. The other way of course, you can also provide energy to the substrate using other means such as light, laser and so on. So you have to be able to provide some source of energy to the substrate.

Typically if the substrate can take high temperatures, thermal energy is the most efficient way to achieve this energization. However there are certain substrates, for example if you are trying to deposit something on aluminum, you really cannot take it to a very high temperature because aluminum will oxidize and form aluminum oxide.

So you have to maintain the temperature not too far above room temperature. But you still need to provide energy to the substrate. Then you have to look at non-thermal means of providing energy to the substrate. In any case, as you design the reactor you have to keep in mind that you have provide an energy source to substrate which is separate from the energy source that you are providing for the entire reactor.

So what are some of the other components you need? You need a vacuum system

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because many reactors, C V D reactors run at reduced pressures. So you have to be able to depressurize the reactor during the C V D process and then re-pressurize it when you are ready to open the reactor and take out the substrate.

And you also need an exhaust system which takes

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the byproducts out of the reactor and by the way this exhaust must be done as quickly as possible because the byproducts are a potential impurity in the C V D film. So you want to minimize the time of contact between the vapor phase byproducts and the film that you are growing on the substrate.

And so the exhaust system has to be extremely efficient. As soon as the byproduct vapors are generated, they must be taken out of the reactor. You also need an exhaust treatment system.

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 \rightarrow Vacuum System
 \rightarrow Cxhaust System

One of the characteristics of C V D reactors is that the byproducts tend to be frequently difficult to handle. You know the byproducts could be chloride, they could be bromides, they could be halides, they could be hydrogen itself or silane, unreacted silane, many of these species are toxic.

So there are lots of environmental and health concerns with byproducts from C V D reactors. And therefore you have to be able to provide appropriate treatment systems to ensure that when the exhaust gases are let out into the atmosphere, they do not have a harmful consequence for people and things in the vicinity. So that has to be built into the system.

And finally as with any chemical reactor, you need a good control system.

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Because it is, especially in the C V D reactor, temperature is a very, very key variable. You

probably require the tightest controls on the temperature distribution in the reactor.

And the second most critical variable is the velocity; the velocity distribution inside the reactor because that is what really delivers the reactants to the substrate and it also takes the exhaust and gets it out of this system. So having tight controls on the transport phenomena inside the reactor is also very important. Of course pressure is important as well. Reactant concentrations, that is another critical variable.And again you have to have separate controls on the substrate temperature versus the reactor temperature. So you need to provide separate control systems.

Many of these reactors also come with in situ inspection systems. That is, as you

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Vacuum System
Jexhaust system incust treatment
control system

make the C V D film you want to assess its quality. You do not want to take it offline, to a lab, wait for analysis to be done and then come back and then if you find out that it is not good, then you might have made another 1000 wafers by then which you have to throw away. So preferably if you can have instrumentation that can look at the wafer in the film as it is growing and do a quick spot check, whether the film is of acceptable quality then your process disruption and cost due to scrap product and so on can be minimized. So it is important to have this in situ inspection system but if you have that, obviously that needs then to be coupled to the control system.

Because as you see things in the film that you don't like, you have to tweak the control parameters so that you bring the properties of the C V D film back to where it should be. So ideally you want to provide almost an endpoint control. As you make a film, you inspect it. If it looks Ok, go. If something looks like it is not where it should be, then you immediately provide a feedback to the system so that the appropriate parameters get adjusted and you bring the process back into line.

And again more advanced manufacturers of microelectronic products where the C V D film characteristics are a very key parameter to control will provide statistical process control. So you do not look at only whether you are meeting or failing a specification but you actually look at how certain critical parameters are deviating from the process mean.

And as soon as the deviations exceed by certain amount, even if you are not failing your spec, you still try to bring it back to its nominal value. So that type of statistical process control and statistical quality control are very critical because these are very expensive operations. The substrates are expensive, the reactants are expensive and the C V D film that you are making is a very valuable thing. You know, you are talking about millions of dollars worth of production on a daily basis. So the control system and the in situ inspection system are very, very key components to the reactor to make sure that we do not waste product. That virtually every product we make is certified to be usable, Ok.

Alright, so these are some of the key parts of the C V D system.

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So what are the key steps in the C V D process? How would you actually run a C V D process?

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Well the first thing that you will do is you have a reactor. So you will first take the substrate on which you are trying to put a film down, mount it on to the load unload mechanism and you will load it into the reactor. You will close the reactor. By the way most C V D systems are run as batch reactors 0:25:24.3. Primarily because the environment of the reactor has to be very tightly controlled. Now there are atmospheric pressure C V D reactors that can potentially be run as flow-through reactors but that is very rarely done.

We will talk about a few cases where that is done, but you know the two requirements to run it as a flow-through process or a continuous process is that the temperatures must not be too far from atmospheric temperature and the pressure must also not be too far from atmospheric pressure, but under atmospheric conditions it is not easy to grow thin films in a controlled manner on a substrate. So it is very rare that we have C V D reactors that are entirely open to the environment.

They are typically operated as close systems with very tight controls on the operating parameters. So as soon as the substrate is mounted into the reactor using the load unload mechanism the reactor is sealed and it is then brought to operating conditions. So temperature needs to be maintained to a certain value. The temperature is increased and you wait until you reach a steady state on the temperature distribution if the pressure has to be modified.

Again you pull the appropriate vacuum and again usually C V D reactors do not run at pressures that are higher than atmospheric pressures but they are frequently run at pressures

that are lower than atmospheric pressure. Can you imagine why? I mean intuitively why would you not want a C V D reactor at elevated pressures?

(Professor – student conversation starts)

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Student: Because of more air, no...

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Professor: The primary reason is that, you will see later that especially at high temperatures, the C V D, the deposition process itself is transport controlled. And the predominant transport mechanism that is happening in a C V D reactor would be diffusion. It is the diffusion across the boundary layer that leads to the formation of the film. And what effect does pressure have on diffusion?

(Professor – student conversation ends)

It is essentially diffusion goes as 1 over pressure, right? So if you go to a high pressure, essentially you will slow down the diffusion process almost entirely. And therefore typically C V D reactors are run at atmospheric pressure or lower.

Ok so you have mounted the substrate, you have brought the temperature and the pressure and all the other conditions to the operating conditions. Then you introduce the reactance into the system and run it for a sufficient amount of time for achieving a certain thickness of the film. The, obviously when you are trying to make any film on a surface, the number 1 metric that you measure is the thickness, right? So when I was talking of the in situ inspection systems what they typically measure is the thickness distribution.

We essentially make the assumption that as long as the thickness on the surface or the film on the surface remains constant the reactor is working in the way it should. Then obviously offline analysis would still be needed to monitor things like impurity levels, and characteristics, you know the metallurgical characteristics of the film and so on but that is not possible to do in situ or online.

So simple online measurement must be as quantitative as possible. It will just give you a number that you can use as an indicator of whether your process is running properly or not. And so the film thickness is typically taken as that variable.

So as you run the reactor, essentially that is what you will do. Once you have brought the reactor to operating conditions you run it for a sufficient number of times, use your inspection system to see whether it has reached the thickness that it has supposed to reach, check for the uniformity of the film and then turn off the reaction.

So the way you do that is you cut off the reactant gases and you bring back the temperature and pressure back to nominal values. And you exhaust the product gases as quickly from the system as possible. So that is typically done using your exhausting system which may simply be again a vacuum pulling of all the species there or it may be a high velocity convector pushing of the product gases out.

So to some extent that depends on the design on the reactor itself. And after the reactants, unreacted materials have been purged from the system then you remove the wafer/vapor from the system and then subject it to further processing or for further analysis and so on.

So that is roughly how you would operate a C V D reactor. But if you look at the deposition process itself, you know what we talked about just now are the various steps in just operating the C V D reactor. But when you look at the formation of the film on the surface, what are the critical steps involved in that? How does it happen? If you look at the C V D process and you break it down into sequential steps what are the different steps that are involved?

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Now from a transport viewpoint, once the gases are introduced into the reactor, the first step is essentially the convective transport of reactants plus carrier gas into the reactor. So again, this needs to stabilize.

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Convective transport of reactants+
Carrier gas into reactor

You need to have the convective flow established in such a way that far from the substrate, we are not talking about flow near the substrate but in the bulk of the reactor we want to establish a stable flow.

By the way in the C V D reactor one thing you must try to avoid at all costs is turbulence. All C V D reactors are designed in order to have laminar conditions of flow inside the reactor. Why is that? Why would turbulence not be desirable? Turbulence has some good properties, right? For one thing it enhances transport rates. Whether you are talking of mass transfer or heat transfer or momentum transfer they are all enhanced when turbulence happens. So why would not you want it? It will speed up the process, right?

(Professor – student conversation starts) Student: uniformity will not be there.

Professor: Yeah, I mean, turbulence by definition is very hard to control.

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If you can achieve controlled turbulence

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then perhaps it is good thing but, I mean, it is just not possible. So while turbulence may offer certain advantages in terms of localized increases in transport rates it is not something you want to have in your system and have to deal with. It is kind of; reverse of stagnation flows, right?

(Professor – student conversation ends)

Why don't you want stagnation flow? Again stagnation essentially implies that there is more time for deposition to happen. The reactants stay in contact with the substrate for a longer period of time, so it is all goodness but then how do you con/control, you cannot control it? Once stagnation happens you cannot break it essentially.

So you cannot have a sharp cutoff and say that this is where I want to stop, you know. As soon as my thickness this number I want to stop here. So you really don't want the two extremes. You don't want the prevailing Reynolds numbers to be so low that you are essentially in creep flow conditions or stagnation conditions. You don't want it to be so high that you are in turbulent conditions.

So you want to operate somewhere in the middle where your Reynolds numbers are reasonably high to ensure that, you know that the convective transport is happening at a sufficiently high rate but at the same time the Reynolds number should not be so high that you kind of slip over into the turbulent region.

The other problem of turbulence is of course is the eddies. You know, once you have these turbulent eddies forming; the transport of material is no more by diffusion. It is essentially whole chunks of fluid are getting thrown around. And so again if you look at a C V D film that has been formed under turbulent conditions it will look very similar to a C V D film that has been formed under homogenous nucleation conditions.

You will essentially have a very, very uneven powdery deposit where certain locations will have essentially 0:34:45.8 whole loads of materials and certain locations will have virtually no deposit. So two things you want to avoid in a C V D reactor, turbulence and homogenous nucleation, Ok.

Ok so the second step is obviously that chemical reactions to happen and these must happen in the bulk phase. When I talk about the bulk what I am talking about is

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ROCES Convective transport of reactants
Carrier gas into reactor
) Chemical reactions to happen in bulk

locations in the gas streams that are very far from the substrate where the deposition is taking place.

You can also call it mean stream, you can call it free stream or we can call it bulk fluid. But whatever term I use, I am basically referring to a location in the gas stream that is sufficiently far away from the substrate. So chemical reactions will continue to happen as long as you have appropriate temperature and pressure conditions.

But in addition we want that chemical reactions must also happen near the substrate and these reactions will be

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qualitatively different from the reactions in the bulk primarily because of the temperature gradient. Because the substrate temperature is different from the bulk temperature, you will form a set of molecules or compounds which are different from the set of compounds that are formed in the bulk fluid. The concentrations will be different.

For example, if S i O H is one of the compounds that is forming, the concentration of that particular compound would be very different in the mean stream condition compared to the near the vicinity of the substrate. It is this concentration gradient that will then drive the transport process, Ok.

So because you have chemical reactions happening in the bulk and the chemical reactions happening near the substrate but under very different temperature and pressure conditions, concentration gradient develops which drives diffusion.

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So the diffusion will happen from bulk fluid to the interface with a substrate but we are still talking about outside the boundary layer.

However as you know when flow happens past a plate, you develop a boundary layer, right? So if the flow is happening in this direction, you will essentially form a boundary layer that looks like that.

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And convective flow will essentially stop when it encounters the boundary layer. The velocities will rapidly decrease. So you still have to transport

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the reactant molecules from just outside the boundary layer to the surface itself. And that has to happen by diffusion across the boundary layer.

And that as I said earlier, is frequently the rate limiting step in a C V D reactor. By the way, diffusion from bulk to the outside the boundary layer is what we call

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4) Diffusion from bulk = interface
5) Diffusion across BL $(*)$

the convective diffusion. So the convection process itself is aiding the diffusion process. So it is essentially enhanced diffusion process. But the diffusion inside the boundary layer is happening in the absence of any convective phenomena. So it is a purely molecular diffusion process which is also aided by something called thermal diffusion.

The existence of the temperature gradient actually induces mass diffusion. We will talk about this later in the course but the combination of thermal diffusion and Fick diffusion actually provides the driving force for transporting the reactant molecules from just outside the boundary layer to the substrate itself. So that is the next step.

So the sixth step would be actual heterogeneous chemical reactions taking place at the substrate which leads to the formation

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) Diffusion from bulk - interface
) Diffusion across BL
6) Heterogeneous reactions at su

of the film, right? So this is the step where we actually start seeing the appearance of a C V D film on the substrate. So that is the sixth step in the process.

Now as the film forms it has to bond to the surface. So the adhesion of the film to the substrate is also very critical step. So in some cases it happens simply by molecular adsorption or molecular attachment. In some cases physical adsorption happens. In some cases chemisorption happens. And obviously the bonding force increases as you go from simple van der Waal's forces of adhesion to adsorption to chemisorption.

And depending on how tightly you want the film to adhere to the substrate you will design the conditions again such that the sticking of the film to the substrate happens by one of these mechanisms. In any case film adhesion to the substrate is also a critical step which again needs to get separate from the deposition of the film.

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4) $Diff_{USion}$ f_{vam} $bdl \rightarrow inferface$

5) $Diff_{USion}$ $aCoSS$ BL

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When you talk about the heterogeneous reactions of the substrate which leads to film formation what you have to keep in mind is that this is a dynamic process. Just because for example, silicon substrate, silicon solid is forming on the substrate does not mean that the silicon is going to stick to the substrate. You still have to provide mechanism by which the silicon atoms that are forming will get attached to the surface. So that is a separate step.

And in fact you can play with the adhesion force by doing things like baking and annealing and so forth. So the initial deposit that forms is actually quite loose on the surface. But as you increase the temperature, as you increase the pressure you can start essentially making it stick much harder.

Sintering is another process that is used to bake the film on to the substrate so that it virtually becomes an irreversible process. Once you have sintered a C V D film on a substrate there is really no, you know chemical means to take it off. You will have to destroy it in order to remove it from the surface.

So what is the other step then? Along with the C V D film that has been adsorbed on the surface you might have some other byproduct gases which have also adsorbed on the surface but these are impurities. So you have to desorb the adsorbed impurities. So desorption of impurities is also an important step.

Desorption of adsorbed impurities, so this ensures the purity

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of the C V D film that you have deposited. Now once the adsorbed species that you don't want have been desorbed, first they have to be removed out of the boundary layer. So you have to kind of reverse the diffusion process. You have to provide an appropriate concentration gradient so that the desorbed species as soon as they leave the substrate will quickly diffuse to the outer edge of the boundary layer.

So the

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exiting of these desorbed impurities from the boundary layer to outside is another important step. Otherwise again they will stick around and keep getting re-adsorbed on to the surface. So as soon as possible you get them out of the boundary layer and then the last step of course is exhaust.

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So all the unreacted gases, all the gaseous byproducts and all the desorbed impurities from the surface all then have to be exhausted from the reactor so that again they do not stick around and re-contaminate your film, Ok.

So if you look at various steps that are involved in the C V D process you get a feel for why, you know, chemical engineering is such an important discipline to apply to the design and operation of a C V D reactor. Each of these steps involves again, either equilibrium thermodynamics or chemical reactions and kinetics or transport phenomena of various kinds, various control mechanisms.

So in order to achieve a C V D film on a surface which sounds, you know, simple enough in principle, you have to pay attention to many of these mechanisms. Each one has the bearing on the next. So it is not that you can kind of design the reactor in sequence. Even though we have broken out the steps in some sequential fashion, I am sure you understand that these are going on simultaneously. So these are highly coupled mechanisms.

Anything you do at a substrate level can even affect even the bulk of the reactor and vice versa. And so whether you are trying to do modeling of C V D reactor or the actual operation, control and optimization of a C V D reactor, you not only have to pay attention to the

individual steps that are involved in the formation of the film but you also have to take a close look at how each step in your mechanism is coupled to the next step and try to obtain a system-wide solution that works for you.

One of the things that I mentioned that somewhat helps us both in terms of modeling as well as operation is the fact that the conditions are typically such that flow is uniform and laminar. And as you know the system becomes much more predictable under those conditions. So you have the potential

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to be able to develop a predictive model for a C V D reactor and

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actually achieve the same results when you actually operate the reactor.

You cannot say that about many reactors in real life. You know, if you go to the chemical industry and you look at the various chemical reacting equipment that are being used, modeling is not first principles based. It is more empirical, data driven. So people collect a lot of data of what is coming in, what is going out and establish correlations. Because really that is the best you can do.

But in a C V D reactor because the conditions are so well-controlled you actually have at least the potential to develop virtually a first principles model and use that for the design of the reactor and the control and optimization of the reactor.

So in subsequent classes we will look at how to develop a good model for a C V D reactor incorporating all these various steps how do you model the thermodynamic behavior of your reactor? When can you assume that equilibrium prevails and when you have to allow for kinetic limitations to kick in? How do you model diffusion processes when there are multiple species that are diffusing? How do you handle the case when there are all dilute species versus the case where some of them are not? How do you take into account the various types of reactor designs?

We still haven't talked about the hot wall, cold wall reactor or the atmospheric pressure, low pressure reactor. There are very, very significant differences in the design and operation of the C V D reactors depending on which particular configuration you go with.

So it is interesting and challenging problem to deal with C V D reactors but keep in mind that, compared to traditional chemical reactors, C V D reactors are run under much more tightly controlled conditions. So you have these ability to apply some of your knowledge about various mechanisms that are prevailing and actually have a practical influence on how the process is run. Ok we will take up some of these aspects in the next few lectures. Any questions on what we have talked about today? Ok, see you then.