

Theoretical concepts in CVD

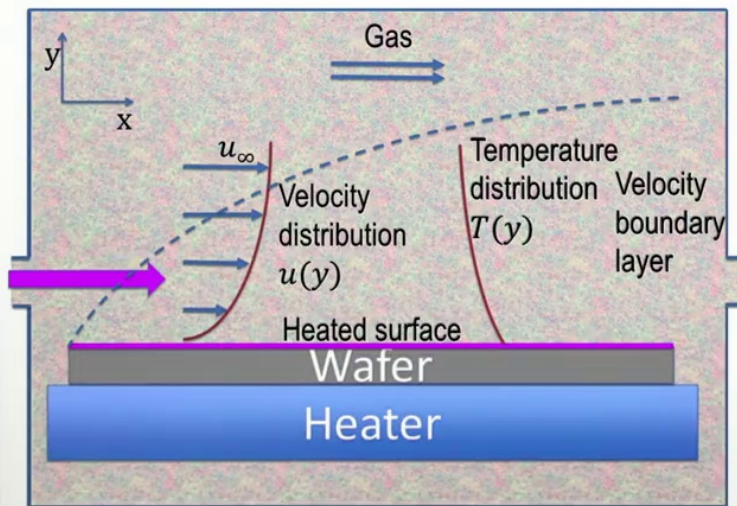


- Velocity boundary layer near a substrate
- Concentration boundary layer near a heated substrate
- Role of the Reynolds number in mass transport

Micro and Nanofabrication (MEMS)

In this lesson, we will introduce some important theoretical concepts that play a role in CVD. These are related to the flow of the gas over the heated substrate. Due to friction forces at the substrate, the velocity is essentially zero, and only when going sufficient distance away from the substrate, when we will reach the velocity of the gas in the free-flow regime. Also, as one consumes gas molecules in the process, the gas concentration at the substrate will be reduced so that there is not only a velocity boundary layer near the substrate, but also a gas concentration boundary layer. Finally, we will introduce how the concept of the Reynolds number plays a role in gas transport over the substrate.

Velocity boundary layer near a substrate

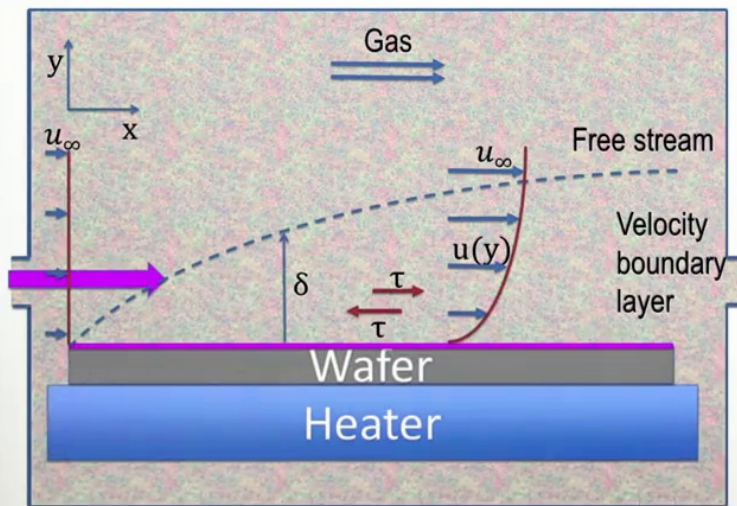


- Gas flowing over a surface at $y=0 \rightarrow$ velocity in the y -direction varies from 0 to value u_∞ at infinity
- Development of **hydrodynamic or velocity boundary layer**
- If temperature gradient, development of **thermal boundary layer**
- **Boundary layer grows** as flow progresses in the x direction

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This slide schematically shows the velocity distribution u as a function of the coordinate y perpendicular to the surface. At the surface, the velocity is zero, and when going up in the y direction, one finds back the free-flow velocity, noted here as u_∞ . This velocity gradient develops in a region close to the substrate, and this region is known as the hydrodynamic or velocity boundary layer. As the wafer is heated, the temperature of the gas close to the wafer will be higher than far away. So there's also a gradient of temperature near the substrate, and this can be associated with the temperature or thermal boundary layer. The boundary layer grows as one advances in the x direction along the flow, as if one goes further, the gas is more and more influenced by layers of gas underneath that have already been perturbed by the viscous flow forces.

Velocity boundary layer near a substrate

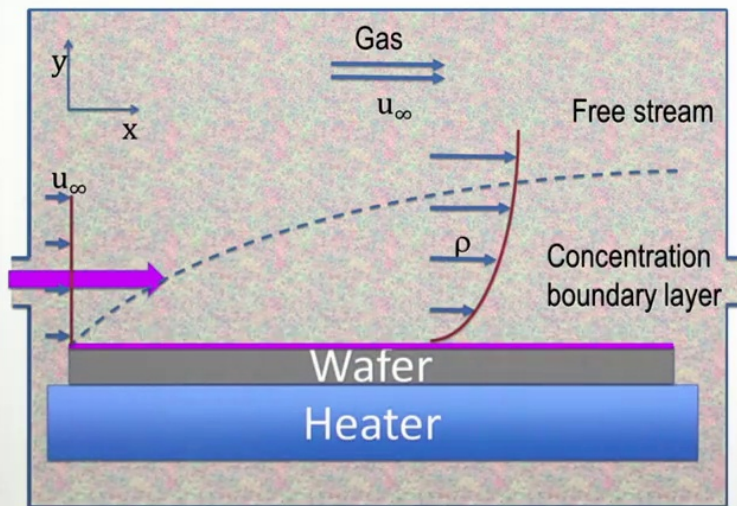


- Retardation of fluid motion associated with **shear stresses** τ acting in planes parallel to the fluid velocity
- $\delta(x)$: **boundary layer thickness**, defined as value for y for which $u(y) = 0.99 u_{\infty}$
- Boundary layer grows with x , as effects of viscosity penetrate further in the gas stream
- **Two distinct regions** in fluid flow: (i) boundary layer where velocity gradients and shear stresses are large; (ii) the region outside, where these are negligible

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Here we show the shear stresses, τ , that act on the gas layer. Shear stresses develop as the velocity of the gas layer underneath is lower than this layer and as the velocity of the gas layer above is higher. The dashed line in this diagram is a theoretical curve which corresponds to the coordinates in space where the velocity of the gas is nearly at equilibrium, that is, nearly u_{∞} . One defines this dashed line as the ensemble of all points where the velocity is 99% of the velocity u_{∞} at infinity. As one goes from the substrate, where there is zero velocity, to this line, where there is 99% of u_{∞} , it is clear that shear stresses are much higher in this region for small x than in this region for high x where the same difference in velocity is developed over a much larger distance.

Concentration boundary layer near heated substrate

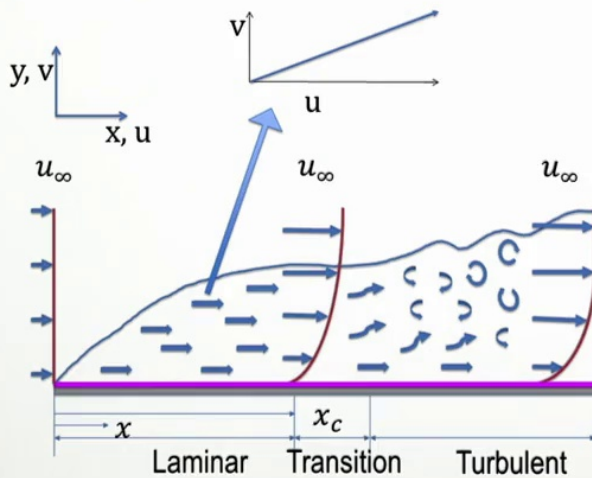


- Gas flows over the wafer surface and is transformed in a solid reaction product
- The gas stream thereby is gradually depleted and a gas concentration gradient $\rho(y,x)$ develops in the boundary layer
- Renewal of the gas from the free stream towards the substrate occurs by diffusion

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This slide shows the concentration boundary layer. During the deposition, due to the consumption of the gas, there is a lower concentration of gas near the wafer. This depletion effect of the gas is counterbalanced by gas flowing from further away by diffusion towards the substrate. In the same way as for the velocity distribution, one can define the concentration boundary layer.

Laminar and turbulent flow

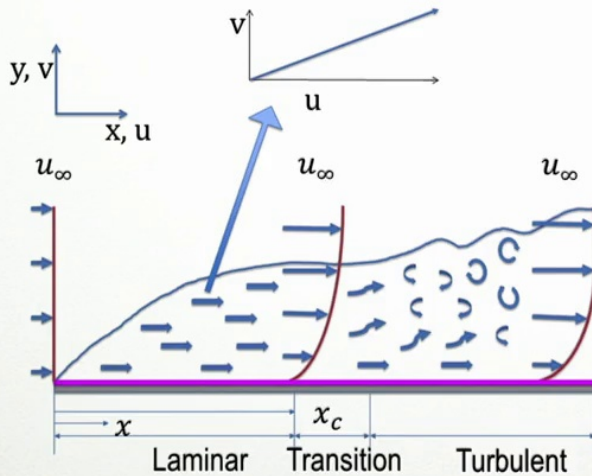


- In general, the boundary layer can be laminar or turbulent
- Laminar
 - fluid motion is highly ordered
 - clear streamlines
 - presence of velocity component v necessitated by boundary layer growth in x direction
- Turbulent
 - irregular flow with velocity fluctuations
 - increased surface friction and turbulent mixing
- CVD is normally operated in the laminar flow boundary layer regime

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In general, two types of flow behavior can be distinguished in the boundary layer. For small x , the velocity is mainly parallel to the x direction due to the high shear forces in the y direction, because we see much bigger shear here where the boundary layer is smaller. For higher x , the thickness of the boundary layer is higher so that the shear forces are less important. In this case, turbulent behavior is seen. Somewhere in between is a critical coordinate x_c where the transition from laminar to turbulent behavior takes place. CVD is normally operated in the laminar flow boundary layer regime where flow is more ordered and regular.

Role of the Reynolds number in mass transport



- The transition between the two regimes is located at x_c and is determined by a critical value of the **Reynolds number**

$$Re_{x,c} \equiv \frac{\rho u_\infty x_c}{\mu}$$

with μ [Pa s] the dynamic viscosity

- For flow over a flat plate, a representative value for $Re_{x,c}$ is

$$Re_{x,c} \equiv \frac{\rho u_\infty x_c}{\mu} = 5 \times 10^5$$

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An important number in hydrodynamics is the Reynolds number which is defined as function of the density of the fluid of the gas in this case, ρ , the velocity denoted by u_∞ and the coordinate along the x direction, x_c . μ is the dynamic viscosity of the gas. Associated with the coordinate x_c , one defines a critical Reynolds number at x_c , and it appears that for all cases, this critical Reynolds number where the transition between laminar and turbulent behavior occurs is at the number 5 times 10 to the fifth. So one can vary density, velocity, or x_c , or μ . Always, the transition will be for this value of the Reynolds number.

Physical interpretation of the Reynolds number

- Re_x may be interpreted as the **ratio of inertia to viscous shear forces** on a gas volume element in the boundary layer

- Inertial force

$$F_i \equiv \frac{\partial[(\rho u)u]}{\partial x} \approx \rho V^2 / L$$

L : system size in the x -direction

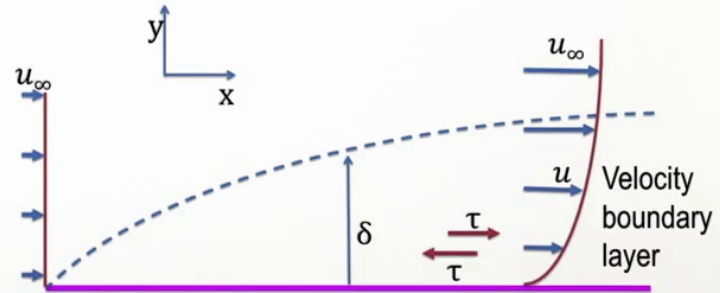
V : mean flow speed

- Shear force

$$F_s \equiv \frac{\partial \tau_{yx}}{\partial y} = \frac{\partial[\mu(\partial u / \partial y)]}{\partial y} \approx \mu V / L^2$$

L : system size in the y -direction

τ_{yx} : shear stress in the x -direction on plane with normal along y



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Here we want to give a physical interpretation of the Reynolds number. It can be thought of as the ratio of inertia to viscous shear forces that act on a gas layer element in the boundary layer. An inertial force per unit volume can be written as the derivative in x of the kinetic energy density, and this can be crudely approximated by this formula: average density, average velocity, and L is the dimension of the system in the x direction. A shear force per volume element or per layer of gas can be written as a derivative with respect to y of the viscous shear forces that act on a plane with normal along the y direction. Again, in a very crude approximation, we can write this shear force by this expression with L , dimension of the system, this time in the y direction.

Physical interpretation of the Reynolds number

- Ratio

$$\frac{F_i}{F_s} \approx \frac{\rho V^2 / L}{\mu V / L^2} = \frac{\rho V L}{\mu} \equiv Re_L$$

- In any flow exist small disturbances that can be amplified to produce turbulent conditions
- For **small Re** , viscous forces are sufficiently large relative to inertia forces to prevent this amplification
- With **increasing Re** , viscous forces become progressively less important relative to inertia forces and small disturbances may be amplified

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Taking the ratio of these two approximative expressions, one obtains this, which is the Reynolds number. This gives us following understanding: In any flow there exist small disturbances that can be amplified to produce turbulent behavior. For small Reynolds number, the viscous forces in the beginning for small x are large enough so that this turbulent behavior cannot develop. With increasing Reynolds number, that means with increasing x , the viscous forces become relatively less important with respect to the inertia forces. As the same difference in velocity develops over the much larger boundary layer in the y direction. Therefore, for increasing x above the x corresponding to the critical Reynolds number, small disturbances may be amplified, and turbulent behavior develops.



- Theoretical concepts of the velocity boundary layer and the concentration boundary layer near a heated substrate
- Role of inertial and viscous forces (Reynolds number) in the boundary layer

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In this lesson, we have seen an important theoretical concept for understanding chemical vapour deposition, namely the development of the velocity boundary layer in the gas and the gas concentration boundary layer near the heated substrate. Also, we mentioned the role of inertial and viscous forces and the Reynolds number for inducing laminar or turbulent behavior of the gas flow in the boundary layer.
