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Design of an automated blade coater &

Design of a gas mixer for a CVD system



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INTERNSHIP CTI - R.G.J. LUBBERS

INTRODUCTION

This report is the result of my internship for my study Mechanical Engineering at the Centre of Technology and Information (CTI) Renato Archer in Campinas, Brazil. During a period of sixteen weeks at the DMI department, I worked at two project: the design of an automated blade coater and the design of a gas mixer for a Chemical Vapour Deposition (CVD) method.

I want to thank all the people that helped me in this internship and my stay in Brazil: Thebano Emílio De Almeida Santos, Fernando Fuzinatto Dall'Agnol, Viviane Carvalho Nogueira, Pablo Jenner Paredez Angelez, Nilsa Toyoko Azana and the rest of my colleagues.

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Muito obrigado!

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SUMMARY

This document contains the reports of two assignments during my internship. The design of an automated blade coater and the design of a gas mixer for a Chemical Vapour Deposition (CVD) system.

The first assignment was to come up with a concept to automate the blade coating process for an OLED on a lab scale. In the current situation the CTI researcher had to use a manual controlled blade coater. For producing a better and more consistent layer every time, an automated blade coater was desirable.

In chapter 1 and 2 the OLED and OLED process are described, followed by the problem definition and list of requirements. Then, several concepts of an automated blade coater are presented and a detailed design can be seen in chapter 9. Here the different functions are explained. The concept is an extra device that pushes the current blade coater forward. In this way no extra costs have to be made to build a new mechanism that holds the blade at the precise position that the current blade coater does. Additional research and engineering has to be done to construct a final design.

The concepts, ideas and possible malfunctions in the blade coating process elaborated in this report have been found very valuable for researcher Nogueira. Fellow student and intern Sjoerd de Bekker continues working on this project after my internship and will make a more detailed design about the automated blade coater.

The second assignment, the design of a gas mixer for a CVD setup, is explained from chapter 10 on. After the description of the CVD process and the current CVD configuration, the problem definition is stated. That is that, in the present setup with a glass basket hanging in the middle of the dome, the process of applying a thin tin dioxide layer on a silicon substrate doesn't provide a uniform thickness. The assignment is to develop a device that mixes the gas mixture better so that a more uniform layer can be applied. Multiple concepts are presented in chapter 14 and the final design, the Static Mixer, can be found after that. A Computational Fluid Dynamic (CFD) analysis has been performed with COMSOL. Its mathematics and the results can be found in chapter 16. In this analysis it can be seen that the designed gas mixer induces a curl in the flows. A 3D printed model is produced and tested at the CTI facility. Unfortunately, the test wasn't a success: the temperature in the CVD installation got too high, causing the gas mixer to melt.

Further research is needed to see if the designed gas mixer performs as intended. Using a different, more heat resistant material, is one of the main recommendations for this assignment.

The references and appendices of both assignments can be found at the end of this report.

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Blade Coating Assignment

The first assignment at the CTI research institute was about a design of a blade coating instrument. This instrument is used to apply an organic layer of a certain thickness to a substrate. This proceeding is used in the process to make OLED (Organic Light Emitting Diode) screens. Currently this instrument is operated by hand and it was my task to investigate the possibilities to automate this process.

The first chapter describes the working principles of OLED screens and after that the process is explained how the OLED samples are made nowadays. Before the different concepts are introduced, the current Blade Coater is clarified. In the end a detailed draft is presented about the final design.

1. OLED

OLED screens are an emerging technology in the display sector. The driving force behind OLED screens is an organic material that emits light when a current passes through. The basic structure of an OLED consists of a stack of organic layers of nanometre thickness between two electrodes, one (transparent)



anode, mostly of indium tin oxide (ITO), and a cathode (metal), see Figure 1. The materials used for the substrate under the anode at CTI are glass and PET. The OLED is finished with a glass plate on top, so that water and air can't get in.

Inside the organic layer electrons are initiated at the (negative) cathode and withdrawn from the (positive) anode. The latter may also be described as the injection of electron holes into the layer. The electrons and electron holes attract each other due to electrostatic forces, forming a bound state: an exciton. The decay of this state results in a relaxation of the energy levels, accompanied by emission of light specific for that material.

Because OLED screens do not need a backlight, it can be thinner and lighter that liquid crystal displays (LCD's). OLED screens can display deep black levels and in low ambient light conditions it can achieve a higher contrast ratio than LCD screens.

The research at CTI concentrates at the production of OLED screens for lightning purposes on a lab scale.

2. OLED PROCESS

The production of OLED surfaces takes place inside gloveboxes, see Figure 3. This is necessary because the organic material should not be contaminated by oxygen or water. Therefore, the room inside the gloveboxes is filled with a mixture of argon and nitrogen gasses at a pressure around 1.6 mbar and a temperature of 20°C. The room is monitored constantly to meet these conditions.

The process starts by making the film. First, the mass of the organic material is weighted and added to the right amount of solvent, in order to make the film with the wanted concentration. The solvents that are used at CTI are chlorobenzene, chloroform, toluene or xylene. Then, it is placed at a shaker to try to dissolve as much as organic material as possible. After that, the film is applied to the substrate using a syringe with a filter.

There are two methods to spread the film over the substrate (dimensions: 50 x 50 x 1 mm). The first is to spin the substrate around, called spin coating. The other method is called blade coating (see Figure 2). Here a straight blade is moved over the substrate. At the moment, this is done manually by using the Blade Coater (see next paragraph), but in the future CTI would like to automate the movement of the blade.





A large disadvantage of the spin coating method is that it causes too much waste of the organic material. And since this material costs around \$ 2.000,- per gram, this can get quite expensive. Therefore the researcher prefers the blade coating method to apply the film of the right thickness. Another advantage of this method is that the roughness of the surface is lower than by using spin coating (1).

Now the substrate is covered with a thin film. The solvent is evaporated on a hot plate which is heated from around 100 °C up till 400 °C. Its dimensions are 210 x 190 x 20 mm. The thickness of the film after

vaporizing the solvent is about 100 nm. These steps can be repeated with different materials if more colours are wanted.

Now, the substrate is moved to another glovebox (the right in Figure 3), one where an evaporator is installed. Here the cathode material is evaporated and attached to the substrate. A mask is used to apply the cathode in a certain configuration.

After this step, the substrate goes back to the first glovebox and an adhesive liquid and a glass plate is attached to the substrate. By using an UV light, the adhesive hardens and the substrate is air and water locked.



Figure 3 CTI Glovebox

The measurements of the OLED's performance also take place inside this glovebox. There are instruments that can measure the light intensity and light spectrum (CIE) of the OLED's.

3. CURRENT BLADE COATER

The current Blade Coater, often denoted as 'doctor blade', is a device that is manually operated, see Figure 4 and Figure 5. The height of the blade can be adjusted using the two micrometres on top. Two springs ensure that the blade is kept at its place against the micrometres. When the mixture of solvent and crystals are at place, one pulls at the handles to make an evenly thick layer on top of the substrate.

The range of height at which the 140 mm width blade can be set is from -2.5 mm till around 11 mm with respect to the subsurface. The blade is at its tip about 1 mm thick (see Figure 5) and can be adjusted quite easily. When the micrometres are set in their most upper position, the blade can be changed. An even wider blade can be mounted in this Blade Coater by changing the two bars to longer ones.



Figure 4 Blade Coater



4. PROBLEM DEFINITION

Figure 5 Cross-sectional view Blade Coater

The CTI researcher prefers the blade coating method above the spin coating method, because there is less (expensive) waste and the roughness of the surface is lower. However, because the Blade Coater is operated manually, this may cause deviations between the various samples. The speed for example can vary from place to place and from time to time.

It is therefore desirable to be independent of the person and to be able to control the movements more precise. Earlier work showed that the speed of the blade is an important parameter for the organic layer and hence the quality of the OLED. In cooperation with the researchers of CTI, the next list of requirements and the conditions has been made.

5. LIST OF REQUIREMENTS

- The horizontal movement of the blade should be automated
- The speed should be adjustable between 5 50 cm/s (± 10%)
- The device should be able to cover substrates with a width of 130 mm
- The height should be adjustable. At least between $30 120 \, \mu m$
- The maximum difference in height between left/right is 10%
- The blade should be exchangeable
- There should be space for the film stock

The process will take place inside the glove box which is kept at room temperatures (20 °C). The table and substrate can be considered flat. The hot plate on the other hand might not. It is expected that the device will be used about 400 times in total. It is not necessary to apply an extra force on the blade since the viscosities of the solvents are very low, comparable with water. However, the moving blade might cause a pile-up of film at corners or a wave in front of the blade. This endorses the importance of having a constant speed of the blade.

In order to get a clear view of the process of blade coating as a whole, different problems that may occur have been listed in appendix A. An overview of possible wear malfunctions can be found in appendix B.

6. CONCEPT PHASE

In this chapter, the concept phase of the assignment is elaborated. First, three different methods of applying the film is described. Then, various solutions to different sub functions are listed.

In general there are three type of methods how to apply the film to the substrate:

- 1. The blade is kept still and the substrate is moving. This is also known as a roll-to-roll process. This method is interesting because of its ability for mass production.
- 2. The substrate is kept still and the *existing* Blade Coater is pushed/pulled over. So, one will need two devices, the current Blade Coater and a new device yet to be designed.
- 3. A complete new design where the substrate is kept still at the hot plate and where the blade passes over. The automated movement of the blade is integrated.

In order to make concepts to automate this process, different sub functions have to be fulfilled. These sub functions are listed in Table 1 below and different solutions are presented to accomplish them.

Function	Solutions	Remarks
Keep substrate at	Noting (just gravity)	
its place		
	Vacuum	
	A ledge	
Change blade	Same as now	
	Slide it in and screw it tight.	
Adapt height	Micrometre(s)	With springs as a counterforce (pull or push)
	Rack	Like in a drill column
Adapt width	Longer rods	
	Different fixation of the blade	Width blade independent of width device
Transmission of	Spindle	
the movement		
	Rack	
	Belt	
Place to push/pull	From 2 sides	Long rod
Blade Coater		2 short rods
	From 1 side	Long rod
	Directly attached to the Blade	
	Coater	
Location of the	Outside the Blade Coater on hot	
base	plate	
	Outside the hot plate	Rigid and straight construction
	Inside of the Blade Coater	Difficult to support and to apply mixture
Guidance	Rods	
	Profile	
	Wheels	

Table 1: Functions and solutions overview

7. CONCEPTS

Based on the list above and information found on the internet, the following four concepts are made. In order to make the right choice between the different concepts, a SWOT analysis (Strengths, Weaknesses, Opportunities and Threats) has been conducted. The results are shown below.

Concept 1: Substrate mover

The first concept uses the first method to apply the film to the substrate. Here substrate is moved, while the blade is kept at a fixed position. The table is moved by using a spindle connected to an electric motor.



Figure 6 Concept 1: Substrate mover

Strengths	Weaknesses
The blade can be fixated rigidly.	The film can slosh because of the moving
Could be placed inside glovebox.	substrate.
	Heating up the substrate is difficult.
	Alignment between blade and table is crucial.
Opportunities	Threats
Experiences can be used for roll-on-roll	Not suited for the small setup in the laboratory.
processes.	

Concept 2: Two Belts Design

These concepts are based on the second method. They use the current Blade Coater and pushes it forward. The difference between these two concepts is that the first (Figure 7) is placed on the hot plate and the second (Figure 8) is placed at the table. The working principle is the same. An electrical engine (illustrated in brown) is driving the two belt. On these belts a rod is attached that pushes the Blade Coater forward.





Figure 7 Concept 2a: Two Belts Design on the hot plate

Figure 8 Concept 2b: Two Belts design at the table

Concept 2: Two Belts Design			
Strengths	Weaknesses		
They have a simple design and therefore cheap	Left and right could wobble		
It uses the current Blade Coater	The Blade Coater must be collected		
Could be placed inside glovebox.			
Opportunities	Threats		
	Only applicable for this process		
	The belt could react with the solvent		

Concept 3: One Belt Design

This third concept is quite similar to the second concepts, only the actuator is on one side. So there's more room to carry out operations inside the glovebox. This concept could be equipped with a blade or only with a rod that pushes the current Blade Coater forward.





Figure 9 Concept 3: One Belt Design

Strengths	Weaknesses	
Enough space to place the film.	Complicated and expensive.	
Possibility to use a longer blade.	The Blade Coater must be collected.	
Could be placed inside glovebox.		
Opportunities	Threats	
Could be used in other processes.	Will need a good guidance.	
	Might need protection for the solvent.	

Concept 4: Blade Mover

This last concept is a whole new device to apply the film of the right thickness. The equipment shown in the images below are quite large, but a further design could be downscaled to an appropriate size for inside the glovebox. This concept is capable of adjusting the height and speed of the moving blade very accurate.



Figure 10 Concept 4: Blade Mover (2)

Concept 4:	Blade Mover	
Strengths	Weaknesses	
Accurate.	Most expensive.	
Fast.		
Opportunities	Threats	
Could be used in other processes.	Too complicated or too large.	
Could be built in an (semi-) automatic	Might need a new glovebox.	
production process.		

8. CONCEPT CHOICE

The final concept of choice is concept number 3, the One Belt Design. A device based on this design has the most potential. Together with the current Blade Coater, a final design is simple and may be used in multiple situations. If the components are mounted to the base in such a way that they can be replaced easily. Then, the device can be used for different applications.

Concept 1, the Substrate Mover, is not suited for the small setup in the laboratories of CTI. It may be an option for future research as an intermediate step, but most likely a roll-to-roll device will be investigated at that time.

Concept 4, the New Blade Design, is too complicated and too expensive for the problem that the researchers are facing.

Despite the simplicity of concept 2, the Two Belts Design, it's not chosen in the end. Mainly because of its limited accessibility and usability. The possible vibrations of the rod or belts of concept 2 is another issue why concept 3 was chosen instead of concept 2.

Looking at the expected costs for each concept, the Two Belts Design is most likely cheaper than concept 1 and 4, but more expensive than concept 2 (see Table 2). The next chapter will show a further developed design of the One Belt concept.

Costs	Concept	
Lowest 2, Two Belt Design		
	3 – One Belt Design	
	1 – Substrate Mover	
Highest	4 – Blade Mover	

Table 2: Order of expected costs

9. DETAILED DESIGN – BLADE MOVER

Based on the ideas of concept 3, the design is developed further. The result, the Blade Mover, can be seen in Figure 11 and inside the setup of the glovebox in Figure 12.



Figure 11 Blade Mover



Figure 12 Blade Mover inside the glovebox

The Blade Mover is actuated by an electric motor (shown in red), that rotates a wheel so that the belt (shown in black) is put in motion. The belt is connected with a sledge by a belt clamp. The 'Top Slider' part is assembled to this sledge and is used to adjust the height. On this 'Top Slider' a rod is mounted that can push the Blade Coater forward. The sledge is guided in one direction by a guidance rail (shown in dark grey).

There is one adjustment that has to be made to the Blade Coater. And that is that on both sides a shackle has to be mounted, see Figure 14. This will ensure that the Blade Coater doesn't fall of the hot plate.



Figure 13 Height adjustment

Figure 14 Blade Coater shackles

In order to estimate the weight of the design and to be able to indicate the power that will be needed for the engine, Table 3 displays the volume and weight (if iron is used) of certain parts.

	Volume (cm^3)	Mass (gram)
Sledge & Top Slider	300	2220
Height assembly	115	851
Blade Coater	183	1354
Total	599	4425

Table 3: Estimated mass properties of the Blade Mover

ENGINE

In order to accelerate the sledge to the appropriate maximum velocity (v_{max}) of 50 cm/s, the engine should be capable of delivering the required force. Based on an estimated total mass that has to be moved and the distances listed below, the necessary force is calculated. The inertia of the wheels and friction is neglected as well as the stiffness of the belt.

Total mass	т	5 kg
Length hot plate		190 mm
Length substrate		130 mm
Length film plate		25 mm
Blade thickness		1 mm
Length acceleration	S	25 mm

The time needed to accelerate the parts till a velocity of 50 cm/s within 25 mm, assuming a linear acceleration is:

$$t_{ac} = \frac{2s}{v_{max}} = 0.1 \, s$$

The necessary force for this acceleration can be calculated by applying the conservation of momentum:

$$F = \frac{m \cdot \Delta v}{\Delta t} = 25 N$$

Since the radius of the centreline of the driveshaft till the centre belt (r) is 26 mm, the theoretical torque needed for the engine to move this estimated total mass has to be at least:

$$T = F \cdot r = 0.65 Nm$$

RECOMMENDATIONS AND FUTURE WORK

The design presented above can be used as a starting point for future development.

One aspect that could improve the design further, is to use a linear motor that has an integrated guidance. These type of motors are commercially available and are an interesting option to look at. This is the most important recommendation to this project.

Furthermore, a final version of the detailed design will need extra attention to certain components. To comprehend the design further, the next aspects can be taken into account:

- Bearings for the axes
- Counterbalance at the other side of the guidance to compensate the moment
- Assemblage (holes, bolts, etc.)
- Tensioner, so that the belt can be put on tension.
- Fixation bolt of the 'Top Slider' part

Design of a gas mixer for a CVD system

10. GAS MIXER ASSIGNMENT

This project is about the design of a gas mixer for a Chemical Vapour Deposition (CVD) system where a coating of tin dioxide (SnO_2) is deposited on a hot silicon substrate. It was found that by using the current setup, shown in Figure 15, the applied coating was not uniform.

In this assignment a possible solution is provided that ensures that the gas mixture is well mixed and that it is spread more evenly across the dome. First the CVD process is described. After that, the current setup is explained, the problem is defined and several concepts are described. The detailed design is followed by a COMSOL analysis and the 3D printed model. After the conclusion at the end, some recommendations are listed.



Figure 15 CTI CVD installation

11. CHEMICAL VAPOUR DEPOSITION PROCESS

Chemical vapour deposition (CVD) is the deposition of a non-volatile solid material onto a heated substrate through decomposition or chemical reaction of compounds contained in the gas passing over the substrate. There are many materials that can be deposited through this process. For example: silicon, carbon fibre, carbon nanofibers, fluorocarbons, filaments, carbon nanotubes, silicon dioxide, silicon-germanium, tungsten, silicon carbide, silicon nitride, silicon oxynitride, titanium nitride (3). Or, as in this case, tin dioxide (SnO_2) .

The depositing material (reactant) should be in the gaseous or vapour phase and react on or near the surface of the substrate, which is at an elevated temperature. This results in a chemical reaction and forms atoms or molecules that are to be deposited on the entire substrate surface. A carrier gas (in this case nitrogen) takes this reactant towards the substrate at the bottom. At CTI, a silicon plate is used as a substrate, which is heated up to 300 °C to 400 °C. The glass wall in this setup is not heated. It is therefore called a cold wall reactor. The temperatures in the bottleneck are estimated between 70 °C and 120 °C.

The basic steps that can occur during the CVD process can be seen in Figure 16.



Figure 16 The basic steps in a CVD process schematically (4)

- (1) Mass transport of the gaseous reactants from the reactor inlet to the deposition zone.
- (2) Chemical reactions in the gas phase leading to new reactive species and by-products.
- (3) Mass transport of the initial reactants and reaction products to the substrate surface.
- (4) Adsorption of these species to the substrate surface.
- (5) Surface diffusion of adsorbed species over the surface to the growth centre.
- (6) Surface reactions at the growth centre.
- (7) Desorption of by-products.
- (8) Diffusive mass transport of the by-products away from the surface.
- (9) Mass transport of the by-products to the outlet of the reactor.

Chemical reaction

The chemical reaction that takes place in order to get the tin dioxide is a complex reaction which is not fully understood yet. There are several chemical reaction that are possible to occur that could realize the deposition of the SnO_2 layer on the substrate. Usually the reaction takes place by oxygenation (equation 1) or hydrogenation (equation 2) of $SnCl_4$:

$$SnCl_4 + O_2 \rightarrow SnO_2 + 2Cl_2 \tag{1}$$

$$SnCl_4 + 2H_2O \rightarrow SnO_2 + 4HCl \tag{2}$$

Both reactions required additional heat to take place, which is realized by the heated substrate. There are many other possible reactions to form SnO_2 , but these will not be treated here.

The chemical reaction between tin tetrachloride $(SnCL_4)$ and methanol (CH_3OH) that could take place in the CVD installation at CTI is (5):

$$SnCl_4 + 4 CH_3OH \rightarrow Sn(OCH_3)_4 + 4 HCl$$
(3)

The formed *HCl* can break down the $Sn(OCH_3)_4$ as follows, forming the tin dioxide:

$$\frac{Sn(OCH_3)_4}{HCl} \rightarrow \frac{SnO_2 + 2 CH_3OCH_3}{HCl}$$
(4)

Additional heat (temperatures above 260 °C) is required in order to let both reactions (3) and (4) take place. A remarkable thing however about reaction (3) is, that in order to break down the methanol,

the presence of a strong acid is needed. This acid isn't present in the reactor and hence the formation of tin dioxide form $SnCl_4$ and CH_3OH remains unclear.

A plausible theory about the chemical process within CTI is that the humidity of the air may take a roll. Since the CVD reactor operates under (normal) atmospheric pressure, the water particles in the air may react according to reaction (2) and play an important role in the whole process. Previous experiments conducted with the same equipment at CTI (5) showed that humidity does have an influence on the reaction taking place. At some levels of humidity, the formation of SnO_2 does not even occur at all. Also the presence of oxygen in the reaction chamber might play a roll.

12. CURRENT CVD CONFIGURATION

Figure 17 shows a cross-sectional exploded view of the current configuration with all the parts. The basket can be seen on the right and in Figure 19. From top till bottom the parts are named are as follows:

- Dome
- Inner ring
- Outer ring
- Substrate support (in red)
- Heater base (in black)
- Foundation

The foundation is the part that is connected to the fume hood's construction. In this part the vacuum pipes are connected to the CVD installation. On top of that is the heater base and heater plate. The heater base contains the heating equipment to heat up the plate with insulation (see Figure 18, left). The heater consists of a resistance heating wire that is embedded in a low conducting ceramic plate to direct the heat towards the substrate's support. The substrate support is a solid stainless steel plate with good heat conducting properties.



Figure 17 Current CVD configuration



Figure 18 Heater and insulation (left) and inner ring with exhaust holes (right)

In the middle of the substrate support a thermocouple is placed to measure its temperature. The temperature of the substrate is assumed to be the same as the substrate's support. This is a valid assumption since the plate has good heat conducting properties and it can store a sufficient amount of heat.

On top of the heater base, the thick walled outer ring and the thinner inner ring part are placed. The latter has eighteen small holes on the inside to ensure that the acid hydrogen chloride can exit the reaction chamber (see Figure 18, right). These holes are the exhaust of the CVD installation. The glass dome is placed on top of the inner ring. At its two inlets, methanol vapour and tin (IV) chloride vapour are introduced in the bottleneck using nitrogen gas as a propellant. The CVD installation uses two bubblers (see Figure 20) to for the inlets. At the methanol inlet, water vapour (or sometimes oxygen) is added to the flow. In the middle of the bottleneck of the glass dome,

there is a glass rod.

In the current configuration a glass basket hangs under this rod, see Figure 19. Its main function is to capture small (tin dioxide) solid particles that appear inside the bottleneck. These particles can cause undesired 'spots' on the coating. It also disrupts the flow to interfere the gas flow and to prevent forced flow reaction.

The mass flow of the two nitrogen flows that enter the reactor vary between 300 and 1000 sccm (standard cubic centimeters per minute) each. Sccm is a volumetrically based mass flow unit which is often used is gas flow measurement. It defines mass in terms of the quantity of gas that occupies a volume under standard conditions of pressure (1.013 bar) and temperature (0 °C) (6).





Figure 20 CVD Bubbler

TIN DIOXIDE

The film that is to be deposited on the silicon substrate is tin (IV) dioxide (SnO_2) . Due to its physical and chemical properties, tin dioxide coatings are used in many applications, like oxidation catalysts, transparent electrodes for displays, touch screens, antireflective coating for solar cells, infrared reflectors, gas sensors, batteries and heating elements (7). The deposition of the tin dioxide at the silicon substrate will start at several places. The final result will therefore be a multi-crystalline coating.

The ratio between the substances in the chemical reaction displayed in equation (4) are never perfect. This is one of the reasons why the tin dioxide layer isn't uniform over the substrate. The dioxide fraction (y) compared to the tin in SnO_{y} , is around 2 and varies from place to place.

The main reason CTI is interested in the tin dioxide coating is because it's transparent and very hard. In future work, the DMI department would like to use it in various optic applications.

13. **PROBLEM DEFINITION**

Producing a silicon substrate with a uniform tin dioxide coating dependents on many factors. Previous measurements showed that by using the current setup, the coating uniformity was not sufficient. One side of the coating was found much thicker than the other side.

To overcome the homogeneity of the flows, research has been done about premixing the flows before they enter the dome. By doing so, the temperature when the mixtures get in contact with each other are lower compared to the dome and hence less likely to react. However, these tests didn't provide the right results. The different components did start to react with each other. Therefore another solution should to be sought.

So, the problem that needs to be solved is:

How can the gas flows inside the dome of the CVD setup be influenced, to optimize the gas mixture for producing a tin dioxide coating on a silicon substrate?

CONCEPT IDEAS

The main idea to influence the flows inside the dome is to design a gas mixer, since adjustments to the glass dome can't be made. The next ideas have been thought of by thinking about the gas mixer in general. The next chapter is more elaborate and specific about different concepts.

There are three functions that need to be fulfilled by the gas mixer. These are the mounting of the gas mixer inside the dome; mixing the gas flows and spreading them evenly over the substrate. One can think of different solutions for these functions:

Mounting

- Using a hook. Similar to the current glass basket
- Using a stopper
- Using a "screw hanger"
- Mounting on the inner ring or hot plate
- Let it hang on the inlets(s)

Mixing

- Active
 Actively mixing the flows: the gases are forced to move by rotating or translating parts
- Passive

Passively mixing the flows: the gases are mixed by static parts that influence the flow directions.

Spreading

- Showerhead
- None. Only using the mixer

14. GAS MIXER CONCEPTS

In this chapter different concepts for the gas mixer are presented. Most of the ideas are based on nowadays products and patents.

An important restriction to the gas mixer is that its design is limited because of the glass rod inside the dome. It is therefore difficult to position additional parts inside the bottleneck.

All the concepts contain passive mixing, since active mixing requires moving parts. In addition, there is very little space inside the bottleneck and changes to the dome can't be made. A detailed drawing of the glass dome with its dimension can be found in Appendix C.

CONCEPT 1: SHOWER HEAD WITH A STOPPER

This concept is based on the head of a shower. Multiple holes divided over two plates, ensure that the gases are well mixed and distributed. If the shower head is able to split, it is possible to try to use different plates for an optimal result.



Figure 21 Shower head

Figure 22 Schematic cross-sectional view shower head (9)

Advantage:

- Possibility to change plates when the shower head can be split
- Reduces the incidence of undesirable spotting and streaking of deposited material

Disadvantages:

- The weight of the design
- Closer to the hot plate, the temperatures get higher. Material properties and thermal expansion should be taken into account

CONCEPT 2A: RAPID MIXER

The Rapid Mixer concept consists of a hollow pipe inside the bottleneck of the glass dome. The gas mixture of $SnCl_4$ in nitrogen is conducted in the outer pipe, the bottleneck. The internal pipe contains the second gas stream, the methanol with nitrogen carrier gas. For a schematic overview, see Figure 23.

The inner pipe includes a mixer tip at the peripheral end thereof. This tip includes a body having an internal passage for conducting the second gas mixture out of the pipe and an opening introducing the second gas stream into the first gas stream in a radial plane at an acute angle relative to the longitudinal axis of the pipe.



Figure 23 Concept 2A: Rapid Mixer (10)

Advantage:

- Mixes the gas mixtures well

Disadvantages:

- Attaching the tubes to the inner pipe
- Mounting the gas mixer in the middle of the glass dome

CONCEPT 2B: SPRAY MIXER

Similar to the Rapid mixer concept, this device has different inlets for the gas mixtures. It is often used to mix gaseous fuel with air for car engines.

Advantage:

- Mixes the gas mixtures well

Disadvantage:

- Connecting the tubes to each other



Figure 24 Concept 2B: Spray Mixer (11)

CONCEPT 3: STATIC MIXER

This Static Mixer concept is based on stationary twisted blades that mix fluids as they pass through, see Figure 25 and Figure 26. This device can be implemented with single or multiple corrugated blades, see Figure 27 and Figure 28.



Advantage:

- Simple design
- Small pressure losses

Disadvantage:

- Difficult to insert in bottleneck

CONCEPT 4: INLINE FIN MIXER WITH A STOPPER

The Inline Fin Mixer concept is a mixer that consists of multiple sets of fins which have such a geometry that they turn the flow inside-out, see Figure 29. The fins are mounted onto a semi cylinder which is attached to a stopper, see Figure 30. In this way the fins can be put inside the bottleneck.



Figure 29 Particle trajectories Inline Fin Mixer (15)



Figure 30 Cross-sectional view Inline Fin Mixer

Advantage:

- Simple design

Disadvantage:

- Doesn't stop undesirable spotting of deposited material

15. FINAL GAS MIXER DESIGN

The final design is a result of the concepts elaborated previously and consists of two parts. The first part is a static mixer, which is composed of components that will influence the flow of the mixture. The second part is a shower head, providing the spreading of the flow. They are mounted together using three small bolts. The design is attached to the glass dome using a screw hanger, which is shown in brown in the figures below.

Above the glass rod, inside the 'bottleneck' of the dome, 10 fins are applied to the static mixer to cause a rotation of the gas mixtures. This curl will improve the mixing of the methanol with the $SnCl_4$. To rotate the gas mixture even further, just below the glass rod, a fin is implemented in the gas mixer. Its 6 blades have to make sure that the flow rotates even more, see Figure 32. At the end, two plates inside the shower head with multiple alternating holes will make sure that the number of spots on the substrate will be reduced to a minimum.

The shower head has to be manufactured in such a way, that it is possible to change the plates. In such a design researchers can vary the number and size of the holes to come to an optimal configuration.



Figure 31 The Gas mixer inside the glass dome

Figure 32 Cross-sectional view Gas mixer

16. COMSOL ANALYSES

To get better insight of the flows inside the CVD installation, a computational fluid dynamics (CFD) analysis has been performed using COMSOL. The total analyses consists of three components. The first and most important component is an analysis of the flow fields of both flows. In the second and third component, the diffusion of methanol and $SnCl_4$ are described.

COMSOL runs three different simulations to calculate the concentrations of methanol and tin tetrachloride. The first is an analysis of the flow field, assuming steady incompressible laminar flow from both inlets. The other two simulations are the calculations of the two concentrations using diffusion-convection equations (DCE).

Mesh

In order to calculate the flows inside the CVD, COMSOL has made a mesh of the domain, see Figure 33. The domain is from the two inlets at the top till the bottom of the gas mixer and it consists of volume elements that do not move. The domain is not extended till the hot plate because there were errors in the simulation of the exits. In addition, the chemical reactions that take place in the lower part of

the CVD are left out of the model. In this way, the simulation focuses only on the changes that are made in the bottleneck of the dome.

ASSUMPTIONS:

There are several assumptions that have been made in order to perform the flow field simulation. Most of them are done in order to reduce the complexity of the problem and to decrease the computational time.



Figure 33 COMSOL mesh of the domain

a) The system is considered stationary.

- **b)** No sources or sinks of mass inside the domain.
- c) Mass diffusion is small compared to mass flow.
- d) No chemical reactions or phase transitions will take place inside the domain.
- e) Volume forces other than gravity are neglected.
- f) The flow is considered incompressible.
 This assumptions is done because the pressure fluctuations are very small.
- g) The viscosity of the system is considered constant.
- h) Uniform temperature (about 100 °C) over the whole domain.
- i) No heat conduction.
- j) No sources or sinks of energy inside the domain.
- k) Flows are of fixed compositions.
- I) Constant diffusion coefficient.
- **m)** No water vapour enters the domain.
- n) Linear flows inside the two inlets.
- **o)** Expansion viscosity is negligible compared with the dynamic viscosity.
- **p)** Newtonian fluids.

MATHEMATICAL BACKGROUND

The CFD analysis of COMSOL uses three basic principles in its calculations. Namely the conservations of mass, momentum and energy. These conservations have to hold for every element in the mesh.

Figure 34 shows an arbitrary moving finite control volume V(t) with closed boundary surface S(t) (also denoted as $\partial V(t)$), which is located at an arbitrary position in three-dimensional space. $\vec{n}(\vec{x},t)$ is the external unit vector normal to the surface, $\vec{u}(\vec{x},t)$ is the velocity vector of the fluid and $\vec{u}_{\partial V}(\vec{x},t)$ is the velocity vector of the boundary. In all the conservation formulas, the higher order terms are neglected.



Figure 34 Finite volume in 3D space

MASS CONSERVATION

The general formula for the conservation of mass is:

$$\frac{\partial}{\partial t} \iiint_{V} \rho\left(\vec{x},t\right) dV + \iint_{\partial V} \left(\rho\left(\vec{x},t\right)\left(\vec{u}(\vec{x},t) - \vec{u}_{\partial V}(\vec{x},t)\right) \cdot \vec{n}(\vec{x},t)\right) dS
= \iiint_{V} \dot{J}\left(\vec{x},t\right) dV - \iint_{\partial V} \left(\vec{J}\left(\vec{x},t\right)\right) \cdot \vec{n}(\vec{x},t) dS$$
(5)

Because of assumption **a**, **b** and **c** the first term at the left hand side and both terms at the right hand side in the general mass conservation are omitted. This will lead to the next continuity equation:

$$\iint_{\partial V} \left(\rho\left(\vec{x},t\right) \left(\vec{u}(\vec{x},t) - \vec{u}_{\partial V}(\vec{x},t) \right) \cdot \vec{n}(\vec{x},t) \right) dS = 0$$
(6)

The only term that remains is the flux of mass out of V.

MOMENTUM CONSERVATION

In addition to the conservation of mass there should be conservation of momentum. The most general form of this equation is:

$$\frac{\partial}{\partial t} \iiint_{V} \rho \,\vec{u} \, dV + \iint_{\partial V} (\rho \,\vec{u} \, (\vec{u} - \vec{u}_{\partial V}) \cdot \vec{n}) \, dS
= \iiint_{V} \rho \,\vec{f} \, dV - \iint_{\partial V} p \cdot \vec{n} \, dS + \iint_{\partial V} \bar{\tau} \cdot \vec{n} \, dS$$
(7)

This formula in fact contains three equations, because momentum has to be conserved in all three directions. Again, the first term is omitted because of assumption **a** (stationary). The external volumetric force field (\vec{f}) is reduced to only the gravitational force vector $\vec{g} = \begin{pmatrix} 0 \\ 0 \\ -g \end{pmatrix}$, assumption **e**.

The result is the next equation for the momentum conservation:

$$\iint_{\partial V} \left(\rho \, \vec{u} \left(\vec{u} - \vec{u}_{\partial V}\right) \cdot \vec{n}\right) dS = \iiint_{V} \rho \, \vec{g} \, dV - \iint_{\partial V} p \cdot \vec{n} \, dS + \iint_{\partial V} \bar{\tau} \cdot \vec{n} \, dS \tag{8}$$

, where p is the pressure and $\overline{\overline{\tau}}$ is the viscous stress tensor. Since the model is assumed to be a Newtonian fluid (assumption **p**), COMSOL uses the next equation for the viscous stress tensor:

$$\bar{\bar{\tau}}(\vec{x},t) = \mu \left[\vec{\nabla} \vec{u} + \left(\vec{\nabla} \vec{u} \right)^T \right] + \lambda \left(\vec{\nabla} \cdot \vec{u} \right) \bar{\bar{I}}$$
(9)

, where μ is the dynamic viscosity coefficient and λ is the expansion viscosity. Because of assumption **o**, the viscous stress tensor can be written as:

$$\bar{\bar{\tau}}(\vec{x},t) = \mu \left[\vec{\nabla} \vec{u} + \left(\vec{\nabla} \vec{u} \right)^T \right]$$
(10)

In this way the viscous stresses depend linearly on the derivatives of the velocity vector.

ENERGY CONSERVATION

The last conservation form that COMSOL uses to calculate the flow field is the first law of thermodynamics: the conservation of energy.

$$\frac{\partial}{\partial t} \iiint_{V} \rho E \, dV + \iint_{\partial V} \rho E[(\vec{u} - \vec{u}_{\delta V}) \cdot \vec{n}] \, dS$$

$$= \iiint_{V} \rho \left[\vec{f} \cdot \vec{u}\right] dV - \iint_{\partial V} p \left[(\vec{u} \cdot \vec{n})\right] dS + \iint_{\partial V} [(\bar{\tau} \cdot \vec{u}) \cdot \vec{n}] dS$$

$$+ \iiint_{V} \dot{Q} \, dV - \iint_{\partial V} [\vec{q} \cdot \vec{n}] dS$$
(11)

The first term is again omitted because of the assumed stationary system (assumption a). In the next term, ρE represents the total energy density which consists of the internal and kinetic energy: $\rho E = e + \frac{1}{2} |\vec{u}|^2$. On the right hand side there will be the rate of work done by the external (gravitational) volumetric force field, followed by the two terms for the rate of work done by surface forces.

The last two terms in equation (11) are omitted because no volumetric heating was assumed (assumption \mathbf{j}) and the temperature was considered constant. So there will be no heat conduction (assumptions \mathbf{h} and \mathbf{i}). The result is:

$$\iint_{\partial V} \rho E[(\vec{u} - \vec{u}_{\delta V}) \cdot \vec{n}] \, dS$$

$$= \iiint_{V} \rho [\vec{g} \cdot \vec{u}] dV - \iint_{\partial V} p [(\vec{u} \cdot \vec{n})] \, dS + \iint_{\partial V} [(\bar{\tau} \cdot \vec{u}) \cdot \vec{n}] dS$$
(12)

Because the flows are assumed to bed of fixed composition (assumption **k**), the thermodynamic state of the fluid is fully determined by two independent thermodynamic quantities. For example the two equations of state $p = p(\rho, T) = \rho RT$ and $e = e(\rho, T) = C_v T$.

DIFFUSION CONVECTION EQUATION

The Diffusion Convection Equation (DCE) is used in the second and third analysis to calculate the concentrations of the methanol and the tin tetrachloride. The general Diffusion Convection Equation is (16):

$$\frac{\partial c}{\partial t} = \nabla \cdot (D \,\nabla c) - \nabla \cdot (\vec{u} \,c) + R \tag{13}$$

c is the species concentration, *D* is the diffusion coefficient, \vec{u} the velocity field and *R* represents the sources or sinks of the species. Again, the first term is neglected because the system is assumed to be stationary (assumption **a**). The last term is omitted as well, because sources/sinks of mass are assumed and in the no chemical reaction is assumed in the concerning domain (assumptions **b** and **d**).

Furthermore, because the diffusion coefficient D is assumed to be constant (assumption I), this parameter can be put out of the divergence operation. And the divergence of the velocity field is omitted as well because of the assumed incompressibility (assumption **f**) of the fluid. This results in the next DCE:

$$D \nabla^2 c - \vec{u} \cdot \nabla c = 0 \tag{14}$$

COMSOL GOVERNING EQUATIONS

Since COMSOL works with the partial differential equations (PDE's) of the conservation laws only, the integral forms (equations (6), (8) and (12)) are rewritten in their differential form by using the theorem of Gauss. The flow field variables must now be continuous. Together with the diffusion convection equation (14), the governing equations that COMSOL uses for the analysis become:

- Continuity equation: $\vec{\nabla} \cdot (\rho \vec{u}) = 0$ (15)Momentum equation: $\vec{\nabla} \cdot (\rho \vec{u} \vec{u}) = \rho \vec{g} \vec{\nabla} p + \vec{\nabla} \cdot \bar{\tau}$ (16)
- Energy equation: $\vec{\nabla} \cdot (\rho E \vec{u}) = \rho(\vec{g} \cdot \vec{u}) - \vec{\nabla}(p \cdot \vec{u}) + \vec{\nabla} \cdot (\bar{\tau} \vec{u}) \quad (17)$ Diffusion convection equation: $D \nabla^2 c - \vec{u} \cdot \nabla c = 0 \quad (18)$

Settings

The parameters that are used for the COMSOL simulations are:

-	Pressure	p = 1 atm
-	Final dynamic viscosity (17)	$\mu = 2 \cdot 10^{-5} \frac{N \cdot s}{m^2}$
-	Diffusion coefficient SnCl ₄	$D_1 = 2 \cdot 10^{-5} \frac{m^2}{s}$
-	Diffusion coefficient methanol	$D_2 = 1 \cdot 10^{-5} \frac{m^2}{s}$
-	Volume flow <i>SnCl</i> ₄	$V_1 = 10 \ \frac{cm^3}{s}$
-	Volume flow methanol	$V_2 = 15 \ \frac{cm^3}{s}$
-	Density SnCl ₄	$\rho_1 = 1 \cdot 10^{-4} \frac{mol}{cm^3}$
-	Density methanol	$\rho_2 = 2 \cdot 10^{-4} \frac{mol}{cm^3}$

The dynamic viscosity that is used corresponds to a temperature of the nitrogen gas around 80 °C. The found diffusion coefficient is of methanol in air at 300 K. The value for $SnCl_4$ is assumed to be the same.

COMSOL RESULTS

Implementing the shower head in the domain led to multiple errors with the boundary conditions. Therefore, and in order to limit the complexity and reduce the computational time needed for the simulations, the analyses is restricted to the Static Mixer.

The CFD analysis performed by COMSOL was executed by an analyst of CTI. He carried out multiple intermediate simulations of the flow field with respect to the dynamic viscosity, to get to the final result. In this way he could check if the flow field was developing as expected. The intermediate results can be seen in the figures below.



Figure 35 Flow field with $\mu = 0.01 \ \frac{N \cdot s}{m^2}$



Figure 37 Flow field with $\mu = 5 \cdot 10^{-5} \frac{N \cdot s}{m^2}$



Figure 36 Flow field with $\mu = 1 \cdot 10^{-4} \frac{N \cdot s}{m^2}$



FLOW FIELD

The final result of the flow field analysis can be seen in Figure 39 and Figure 40. This simulation is performed with a dynamic viscosity of $\mu = 2 \cdot 10^{-5} \frac{N \cdot s}{m^2}$.

The arrows in Figure 40 indicate the direction and magnitude of the flow. However, there is a logarithm function applied to the arrows. Some whirling can be noticed as well as some back flux.



Figure 39 Flow field with dynamic viscosity $\mu = 2 \cdot 10^{-5} \, \frac{N \cdot s}{m^2}$



Figure 40 Flow field inside the Static Mixer





CONCENTRATION PROFILES

As described in previously, the flow field is used together with the Diffusion Convection Equation to calculate the concentrations of the methanol and $SnCl_4$. The result of these two simulations are displayed in Figure 41 and Figure 42.

The concentration profile of $SnCl_4$ in Figure 41 shows that the maximum difference in concentration is 33%. The maximum difference of methanol is 42%. The influence of the glass rod in the middle of the bottleneck can clearly be seen.



Figure 41 Concentration of ${\rm SnCl}_4$ at the bottom of the Static Mixer



Figure 42 Concentration of methanol at the bottom of the Static Mixer

17. 3D MODEL STATIC MIXER

To investigate the design in reality, a 3D printed model of the mixer is produced. The material that has been used to fabricate this model is Polyamide (PA12), a nylon polymer. It is a suitable material for this application, because it is easy to fabricate and it doesn't react with methanol and $SnCl_4$. A cross-sectional view of the Static mixer and the 3D printed model can be seen in Figure 43 Cross-sectional view Static Mixer and Figure 44 respectively.

The used 3D printer at CTI has an accuracy of 0.1 mm in z-direction and it has a resolution of 0.8 mm in x- and y-direction. There we no restrictions in the model geometry and no support structures needed to be added. However, the model had to be manually sanded to fit exactly inside the dome.



Figure 43 Cross-sectional view Static Mixer



Figure 44 3D Printed model Static Mixer

18. TEST RESULTS

Unfortunately the test didn't go as planned. After the first test was carried out, one could clearly see that the setup had failed. The temperatures at the bottom of the bottleneck of the glass dome became much higher than estimated in advance. As can be seen in Figure 47 and Figure 48, the polyamide bottom of the Static Mixer got degraded.

The positioning of the 3D printed Static Mixer inside the glass dome is shown in Figure 45 and Figure 46.



Figure 45 The Static Mixer inside the glass dome



Figure 46 Bottom view Static Mixer



Figure 47 Inside view of the Static Mixer after the first test



Figure 48 Outside view of the Static Mixer after the first test

19. CONCLUSION

The COMSOL analysis of the flow field show that the Static Mixer causes a curl in the flow field inside the bottleneck of the glass dome as well as some back flux. From the concentration profiles can be concluded that the introduced curl slightly influences the concentrations of both the tin tetrachloride and methanol. But the diffusion seem to be the most important factor.

Unfortunately, the test inside the CVD with the 3D printed model didn't provide any useful results. But from the COMSOL analysis can be concluded that the designed Static Mixer is an improvement with respect to the previous glass basket. The mixer makes sure that there will be a small rotation of the flow that previously wasn't there.

If the suggested Shower Head is installed as well, an improvement in uniformity of the tin dioxide coating is most likely. Possible solid particles will be collected as well. Further tests will have to show if the uniformity will be sufficient.

20. RECOMMENDATIONS

Using the current configuration there are several aspects that could be worth investigating. Both about the COMSOL analysis and about the 3D printed model that has been used.

- Investigate the Static Mixer design using a material that is heat resistant, like a ceramic or metal.
- Investigate the use of a Shower Head. This part can be attached to the Static Mixer or, it could be a disk that is laid on the Inner Ring of the CVD installation.
- Optimize the Static Mixer. So more/different blades could be placed in the first part and in the fan in the middle.
- The temperature control of the heating plate could be insufficient since there is no feedback of the temperature of the plate.
- Use a more representative dynamic viscosity in the simulations: Diffusion coefficient of methanol in nitrogen at 300 K (18) $D = 14 \cdot 10^{-6} \frac{m^2}{s}$

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22. APPENDIXES

A. BLADE COATING PROBLEMS

List of potential problems in the process:

- The substrate moves away
- The blade has an inclination
- The blade wobbles while moved (right and left side have different speed)
- The blade lifts up
- The blade tilts
- The blade shifts from left to right inside its 'chamber'
- The blade moves forward/backward
- The power and torque of the engine should be sufficient (maybe an extra transmission is needed)
- The pressure exerted by the blade on the film should be sufficient
- The film shows a sort of wave
- Beside pushing/pulling the Blade Coater forward, you also have to slow it down or collect it to prevent it from falling of the hot plate
- Attach the device to the hot plate (for example a sort of hook/bolt or shackles). To prevent the device from slide while moving the blade forward
- The place of the substrate on the hot plate may affect the end result
- A proper fixation of a rod/piece to a belt
- Ability to delay the start (in order to keep it steady / hold it still)
- Changing the width (or other dimensions) should be easy
- Assembling the device should go easy

Out of this scope:

- The speed at which the solvent is evaporated is crucial
- The ground / hot plate / substrate is not straight (oxide layer for example)
- The temperature of the hot plate is not uniform
- The variation of the thickness or roughness of the substrate is too high
- The amount of crystals in the solvent should be sufficient for the desired thickness of the layer
- The crystals should be well solved in the solvent and small bits should be filtered out
- Substrate material (glass, silicon, ...)

B. BLADE MALFUNCTIONS

List of blade wear (19):

Troubleshooting — Blade Wear Identification



C. CROSS-SECTIONAL VIEW GLASS DOME

The figure below shows the cross-sectional view of the modelled glass dome with all its dimensions.

