IMEC

Designing a Heating Element for a CVD Reactor

Caitlin Brown, Yonathan Hodish, Son Pham, Lamisa Sharmin, Joshua Habash

The Company

For our senior design project, we were assigned to work with the Interuniversity Microelectronics Centre, IMEC, to design a heating element in a chemical vapor deposition reactor for a silicon wafer. IMEC, founded in the 1980s, is a medium sized company headquartered in Leuven Belgium. They are involved in a number of industries including the life sciences, telecommunications, and the automotive industry. Our project focuses on semiconductors which aligns with the company's involvement in the nanoelectronics industry.

Company Business

This project is important for IMEC as the company wants to scale down the dimensions of logic devices and explore new paths on the system level. The size of semiconductor chips is getting smaller over time with increased efficiency and performance. However, simply downsizing the pattern of integrated circuits does not lead to beneficial achievements, and minimizing the size of semiconductors will lead to exceeding physical limits. In other words, downsizing semiconductors for efficiency purposes will require more developed manufacturing processes that have to both decrease energy consumption and assure environmental safety.

Furthermore, since the world is becoming more solar-energy-focused, thin film solar cells are crucial in order to maximize energy efficiency and sustainability. As these CVD reactors are commonly used in the microelectronics industry, they are utilized to apply thin layers of materials, such as GaAs, CdTe, Crystalline Si, and Perovskite materials that are present in solar panels. Also, since CVD is an integral process in making semiconductor products, it helps IMEC achieve the goals for high-end CPUs and GPUs [1].

Chemical Vapor Deposition

Chemical Vapor Deposition, CVD, is the process of placing a uniform layer of a metallic substance through the application of a gaseous mixture of the metal. The process requires very high temperatures, greater than 1000°C, and a vacuum environment, however we were instructed to proceed as if the reactor was approximately at atmospheric pressure. We need to design a heating element for a CVD reactor that would facilitate the deposition of gallium nitride (GaN) on silicon wafers. Below is the chemical reaction of the process:

$$Ga_2[N(CH_3)_2]_6 + 2NH_3 \rightarrow 2GaN + 6HN(CH_3)_2$$

This suggests that in the thermal depositions, NH_3 undergoes transamination reactions with the dimethylamido compounds, which replaces the dimethylamido ligands with dimethylamine and gets the precursor out of carbon-containing groups. Although the metal precursors have nitrogen containing ligands, NH_3 is necessary to minimize carbon contamination [2].

Chemical Vapor Deposition involves several elaborate reaction supporting equipment such as the showerhead dispenser, vacuum system, and a heating element. Our project focused on the heating element. The specifications were to have it heat the wafer uniformly, having a temperature difference no more than one degree celsius across the wafer, to 1,100℃.

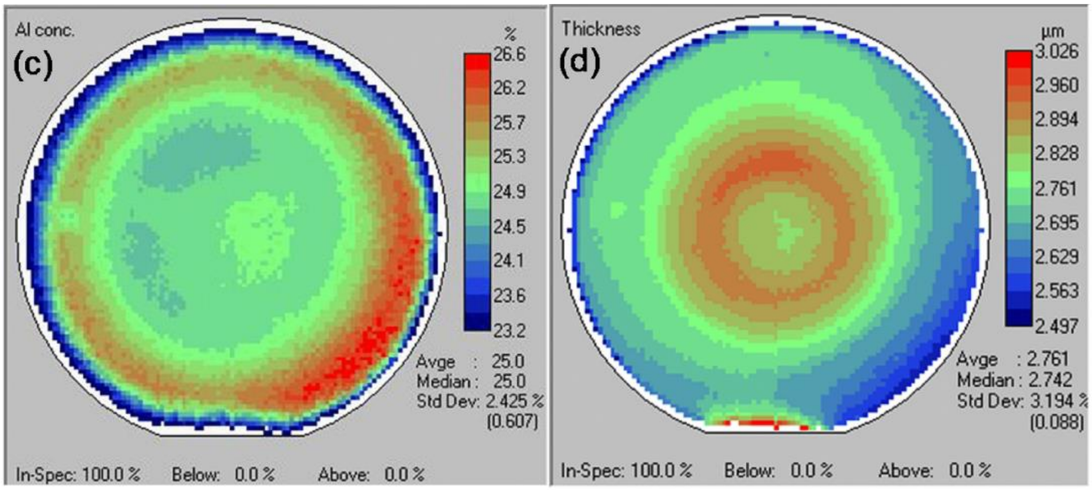


Figure 1. A photoluminescence (c) and thickness (d) map of the aluminum gallium nitride deposition on a wafer from a publication on findings in CVD. This paper introduced us to the topic of CVD.

Chemical Vapor Deposition is a profound method that is commonly used to deposit a layer of material ranging from nano- to micrometers thick on wafers. Chemical Vapor Deposition process takes place in a CVD reactor. There are various kinds of CVD reactors depending on what pressure they operate at, flow of gasses in them, the source of energy used, wafer orientation, and other factors. In this project, we will focus on designing the heating element of a vertical disk type of CVD reactor shown in the figure below.

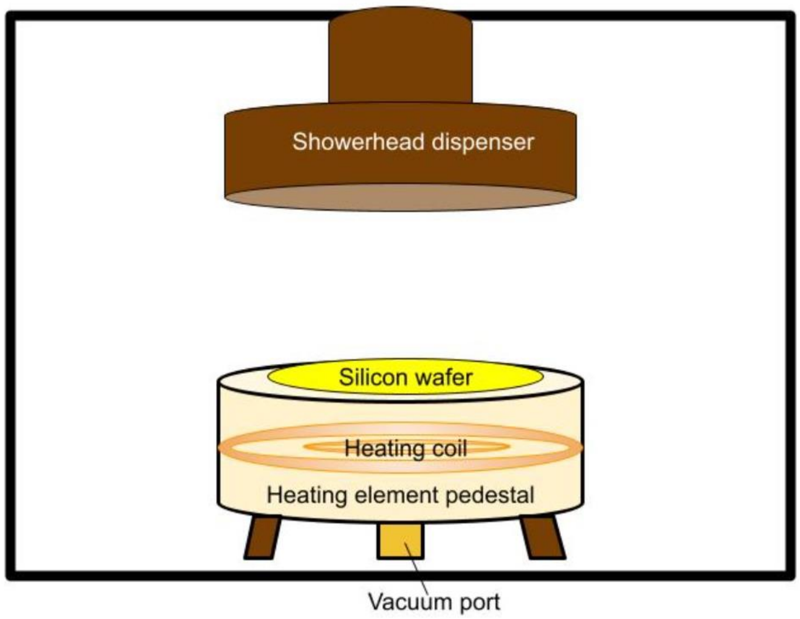


Figure 2. A simplified diagram of a CVD reactor.

The main parts of this reactor are:

- Showerhead dispenser - this is entry point of the precursor gases into the reactor
- Reactor walls - enclose and seal the reactor to prevent the leakage of gases and IR radiation from the reactor to the surroundings
- heating element - gives support to the silicon wafer as well as heats up the wafer to the desired temperature for deposition to take place
- Vacuum port - holds the wafer firmly on the heating element

In this project, we only focused on designing the heating element of the CVD reactor such that it heats up the silicon wafer uniformly to a set temperature for the deposition of a gallium nitride layer.

Source of Heating

Joule/resistive heating was the method used to provide heat in the CVD reactor. Joule heating refers to the thermal energy produced as a result of passing an electric current through a conductor. The heating element of the CVD reactor will contain a coil embedded in it. Passing an electric current through the coil will produce the thermal energy required to heat up the wafer to the required temperature. Our goal is to achieve a uniform temperature distribution throughout the surface of the wafer in order to deposit a layer of uniform thickness.

The first step in designing this heating element was to recognize the factors that would affect temperature distribution. The variables that were tested in the design of this heating element were:

- Number of coils and the spacing between them
- Coil configuration (concentric circles or spiral)
- Coil cross-section and size
- Material choices (what the coils, insulation, and substrate layers are made of)

Designing the Heating Element.

The preliminary steps we took in designing this heating element were to make 2D heat transfer models on a simulation software known as COMSOL Multiphysics. These 2D simulation models helped us understand how the above mentioned variables would affect temperature distribution on the surface of the wafer.

For instance, when looking at the spacing between the coils, having few coils that were spaced far apart resulted in hot spots. We needed to add more coils to even the temperature distribution. We evaluated which design used the least amount of turns in the coil, but still heated the wafer uniformly. We started with coils with square cross-section because they had better contact with the wafer suspender and thus provided better heat transfer. However, we later decided to proceed with circular cross-section coils because coils with cylindrical geometry would be easier to manufacture and thus economically favorable. **Figure 3** below shows one of the 2D model where we tested the effect of the spacing between the coils.

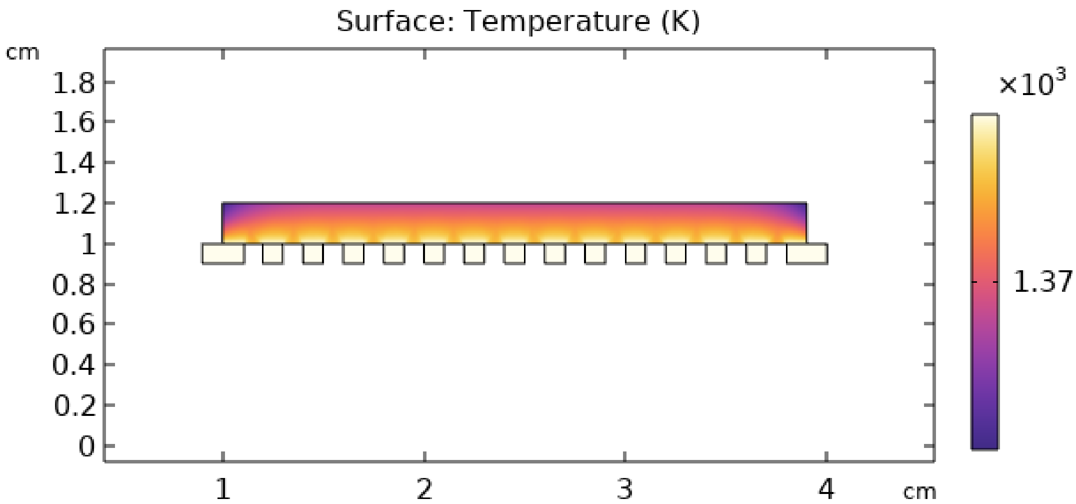


Figure 3. 2D model of temperature distribution from coils to wafer suspender

The choice of materials to be used for different parts of the heating element was the next crucial phase of the design process. We needed to find the appropriate materials for the coils, insulating layer, and the wafer suspender. These materials were supposed to be not only functional but also economically favorable. The coil had to be made from a material that could withstand very high temperatures (>1000 ℃). An insulating layer around the coils was added to protect the reactor from the extremely high temperatures of the coils. The insulating layer had to be made from a material that could hold the coils and also prevent the thermal energy generated from going into unwanted regions. The wafer suspender had to be made from a material that could smoothly transfer heat from the coils to the wafer. We studied past publications to learn what were the commonly used materials in CVD reactors. Pyrolytic boron nitride was chosen for the coil insulating layer. Pyrolytic graphite was chosen for the coils themselves. Graphite was chosen to make the wafer suspender.

After learning about the effects of the different variables on temperature distribution from the 2D models, and the appropriate materials to use for the different parts of the heating element, we were able to perform a higher-level simulation model. A 2D-axisymmetric model on COMSOL allowed us to perform a 3D simulation.

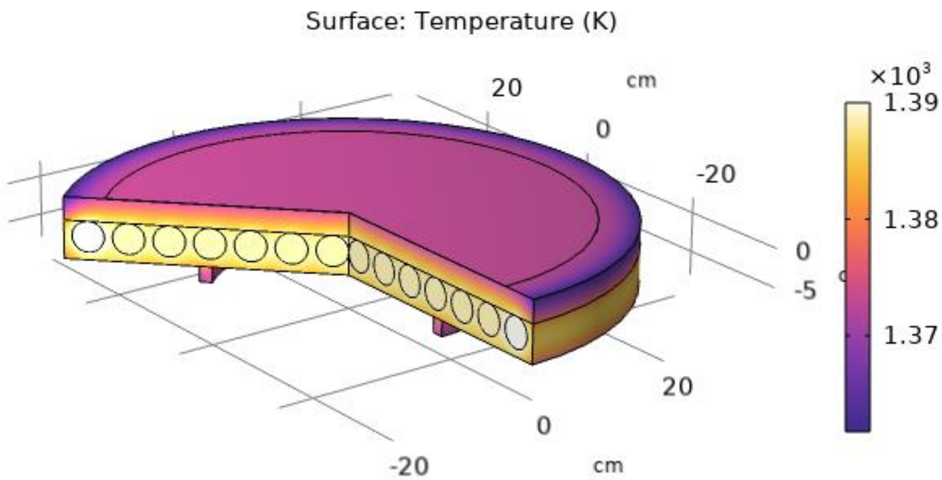


Figure 4. First 2D Axisymmetric model

This model reached specifications and had the wafer have a surface temperature between 1100 and 1099.7℃. It consisted of one coil with six rotations and one outermost ring. The outer ring was heated to a higher temperature. This alleviated the problem of the edges of the wafer becoming much colder than the interior.

The model would be practical to implement, however we failed to consider the safety of a 4 cm diameter wire with resistance heating. The current required to generate the required heat in this scenario would be extremely large and most likely unsafe. This led us to adjust the design to utilize a more realistic wire diameter.

Solution: The Final Product

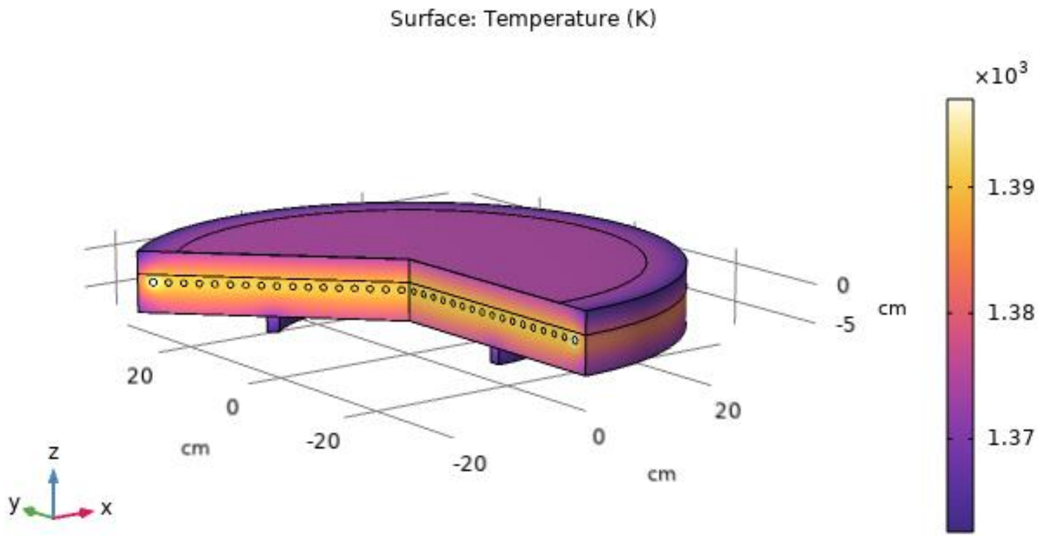


Figure 5. Final design of heating element

Our final design consisted of a heating element on which a 30 cm wafer is placed. One coil is wrapped around to create 16 cross section points on each side of the cylinder cross section. An outer ring is placed around the coil. This ring has a larger diameter of 0.93 cm in contrast to the coil diameter of 0.83 cm. It is also heated to a higher temperature than the coil to accommodate for the issue of heating up the cold edges of the graphite holder.

As shown in **Figure 5**, we achieved a uniform heating pattern. This is within our target temperature range which results in a uniform deposition layer onto the wafer. Comsol used the following equations of convective heat transfer to generate the model in **Figure 5**:

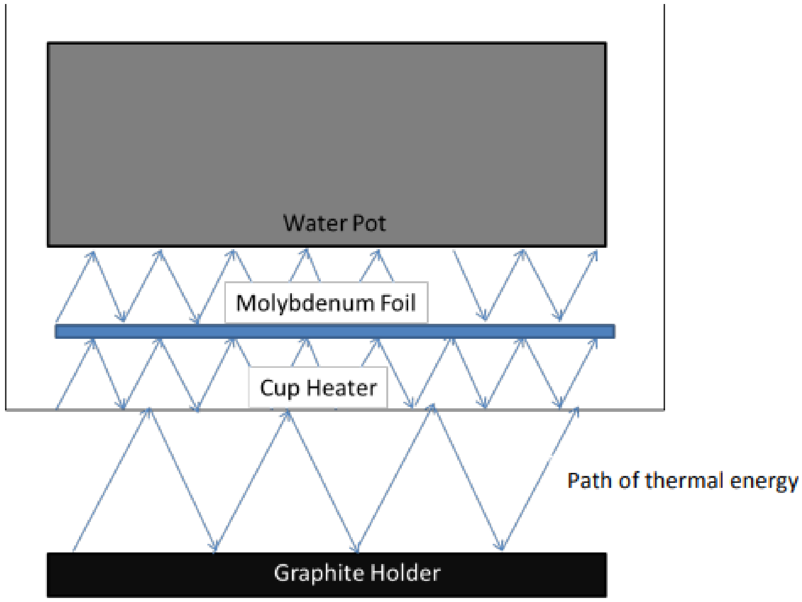
$$\rho C_p u \cdot \nabla T + \nabla \cdot q = Q + Q_{ted}$$

$$q = -k \cdot \nabla T$$

The variables are defined as follows: ρ is the density in kg/m^3, C_p is the specific heat of the material in J/(kg・K), u is velocity in m/s, q is the conductive heat flux in W/m^2, Q is the heat source in W/m^3, Q_{ted} is the thermoelastic damping in W/m^3, ∇T is the temperature gradient in Kelvin, and k is the thermal conductivity in W/(m・K). Each material has different properties such as thermal conductivity and specific heat.

Using the equation of enthalpy:

$$\Delta H = -c \cdot m \cdot \Delta T$$



We calculated the amount of energy generated by the current running through the graphite coils. We calculated the energy requirement to be 10^6 J, however the difficult part was in determining the power requirement, or the wattage. The heater power output and operating duration depended on the deposition reaction and conditions within the reactor chamber (such as temperature and pressure). Regardless of the duration, the cost required to operate the heater is insignificant compared to the value of the product being made.

Due to time limitations on the project, we could not design a cooling system for the heater, however the following design has important features that we would need to consider. At these temperatures, graphite coils emit infrared (IR) radiation. Heat is now transferred via radiation, which can travel through vacuum and could lead to a reactor meltdown.

Figure 6. Diagram of a CVD cup heater (Points, 2013). The cup heater in the thesis uses thermal radiation as the primary means of heating the graphite holder. The water pot is chilled and encased by stainless steel (SS).

A similar cooling mechanism as in **Figure 6** could be implemented with our heater, however since our primary heating mechanism is conductive and not thermal radiation, a metal that has higher absorbance would be more fitting as a protective measure against reactor meltdown.

Economic Analysis

The three main factors we originally considered when thinking about economic tradeoffs include diameter of heating coils, choices of materials used, and energy consumption of the heater. One of our initial models (Fig. 4) contained coils with a 4 cm diameter. After running the model, we concluded that such a diameter was too heat intensive and required coils not widely manufactured in that size (due to safety of current). Thermal stability was the main factor driving our choice of materials for the heating element. We focused on prioritizing functionality to produce the most uniform heat layer in our model (Fig. 5). Our final model had an insignificant power requirement in comparison to the value of the product being produced.

Safety and Environmental Considerations

When considering the safety and ethical implications of our design, one main safety precaution that will be incorporated into our design is grounding the system in order to subside destruction in the event of a power surge or equipment failure. Our design will require the addition of a metal cord contacting the base of the heating coils that extends to a grounded metal surface outside of the reactor. Without this grounding, the circuits could be rendered destructive during power surges and/or equipment failure.

Gas leakage from the reactor sealing layer is another safety concern in our design. The CVD reactor could incorporate some forms of gas sensors that would be able to detect if any gases from the reactor are leaking into the surroundings. Then, appropriate measures such as evacuating and venting the reactor should be taken in order to minimize the risk of exposing workers to those harmful gases. CVD requires volatile metallic-organic precursors that can be toxic, corrosive, or explosive. After deposition, the byproducts of the reaction also can be dangerous, for example hydrofluoric acid. This vapor and any components transferring it must be secured thoroughly to prevent hazardous leaks. In order to prevent gas leakages, the reactor pressure should be kept under the atmospheric pressure. At the same time, the gas flow rate must also be controlled in correlation with the pressure change during the reaction. Due to the sealing layer operating at high temperatures that may alter the pressure of the system, there is a possibility of gas leakage occurring from the changes in pressure. To ensure safety and avoid gas leakages, it is important to make sure the CVD system is leak tight during the pump-fill cycles before switching to process gas. Additionally, it is beneficial to consider implementing an internal alarm within the system to detect fumes and gas leaks which can then, in response, automatically alter the pressure back to a stable state and alert all workers of the possible leak.

As for environmental implications, the primary precursors of boron nitride are boron and ammonia. While ammonia production is somewhat benign, in 2019 it produced more carbon dioxide emissions than any other chemical making reaction. A bigger concern for our heater design is boron nitride. Boron mining practices are environmentally destructive. Mining of boron not only requires large amounts of water, but degrades the landscape and can destroy wildlife habitats permanently. It is very important to be mindful of where this mining is occurring and making sure it is not destroying habitats and away from wildlife. It is also very important to note that the locations usually used for boron mining are in arid climates in which water is already very scarce and crucial for not only the community but the wildlife and survival of many different species. Boron is extracted in open-pit mines by drilling, blasting, crushing and hauling which are all activities that are fueled by petrochemicals. This refining process then uses a significant amount of water. Boron mining pollutes not only the air but the water, making it unusable for any source of consumption due to the high levels of toxicity in the water.

Overall, while the semiconductor industry does consume high amounts of energy and releases significant amounts of waste, the industry itself also has many benefits including enabling technologies critical to U.S. economic growth, national security, and global competitiveness. Because most semiconductor devices also have unlimited life, this can in the long run, reduce material waste while advancing to reduce the energy required to run these devices.

Challenges of GaN on Si

Despite the cost advantages of using Si as the material has been used for various applications, the physical properties of GaN and Si in a way that creates two major problems that need to be addressed. The first challenge is that the GaN/Si interface will lead to an eutectic reaction that can happen at a very low temperature relative to growth temperatures, which results in Ga meltback etching of the Si substrate. The other hurdle that is needed to be overcome results from the different crystal structure of Si and GaN. While Si has a face-centered cubic crystal, GaN has a hexagonal wurtzite crystal that when the two materials being coupled together will lead to large mismatches between lattice parameters and thermal expansion coefficients. Such differences will often create high tensile strain in the GaN epilayers that further increases the defect densities and cracks on the thin films [3].

Limitations in Our Design and Suggestions for Improvements

Given the resources and time limitations, we could only focus on designing one part of the CVD reactor, the heating element. With this approach followed, the resulting designed solution was only a part of a whole. Some of the limitations of our design due to the approach we took included the software used, the information available to us, and the disregard of infrared radiation (IR).

COMSOL Multiphysics is an elementary physics engine. It is not used in precise, real world applications because it does not evaluate enough physics phenomena present in the real world. The computations are surface level and without a more comprehensive software, this design is only a rough estimate.

Although we only focused on designing the heating element of the CVD reactor, designing a system for radiative heat loss mitigation is also very important. The next step would be designing mechanisms to properly cool the CVD reactor as well as shield the emitted IR radiation from leaking into the surroundings.

References

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