CHAPTER 2

LITERATURE REVIEW

2.1 History of the CVD processes

CVD reactors have been around since the early twentieth century, with the earliest patents for CVD processes being filed in the 1920s and 1930s. However, the early CVD processes were not very efficient and were mainly used for the production of speciality chemicals (Pierson, 1999). In the 1950s and 1960s, advances in the understanding of the chemistry of CVD reactions and the development of new reactor designs led to the commercialization of CVD for the production of thin films, such as silicon dioxide and silicon nitride, for use in the semiconductor industry. During the 1970s and 1980s, CVD reactors became increasingly sophisticated, with the development of new reactor designs such as horizontal and vertical tube reactors, and the use of computer control systems to optimize process conditions. In the 1990s and 2000s, CVD was used for the growth of a wide range of thin films, including those made of oxide, nitride, and carbide materials for use in the semiconductor, optical, and biomedical industries (Sun et al., 2021). Furthermore, new reactor designs, such as atomic layer deposition (ALD) and molecular beam epitaxy (MBE), have been developed to enable the development of high-quality thin films with precise control over film thickness and composition (Oke and Jen, 2022). Today, CVD is a well-established technique and is used in the production of a wide range of products, including electronic devices, solar cells, and biomedical implants.

2.2 Modelling approaches in CVD

Parametric modelling approaches refer to the methods used to develop mathematical models that describe the relationships between process parameters and the desired outcomes. These models help in understanding and predicting the behaviour of the CVD process, enabling optimization and control. Here are some commonly used parametric modelling approaches in CVD (W Benzinger et al., 1996; Gupta et al., 2022b; Hu and Hüttinger, 2001; Lacroix et al., 2010; Lin et al., 2009a; Meshot et al., 2020; Shinde and Pradeep, 2021)

1. **Empirical models:** Experimental data and statistical analysis are used to build empirical models. They entail using data-driven methodologies to find patterns and

connections between process parameters and outcomes. To represent the correlations between variables, empirical models may employ regression analysis, response surface technique, or artificial neural networks (Chen, 2007; Kober et al., 2022).

2. **Semi-empirical models:** Semi-empirical models combine empirical observations with some underlying physical principles. These models incorporate a mix of empirical data and simplified mathematical representations of the physical and chemical processes involved in CVD. Semi-empirical models are useful when the underlying mechanisms are partially understood but may still require some empirical adjustments (Chuang and Chen, 2014; Filho et al., 2020).

3. **Kinetic models:** Kinetic models focus on the chemical reactions and kinetics occurring during the CVD process. They entail quantitatively characterising the rates of specific reactions and their relationships to variables like as temperature, pressure, and reactant concentrations. Kinetic models can be used to simulate chemical reactions on the surface and in the gas phase using reaction rate equations, mass transfer equations, and thermodynamic principles (Benzinger et al., 1996; Gupta et al., 2022b).

4. **Computational fluid dynamics (CFD) models:** CFD models solve the governing equations of fluid flow, heat transfer, and species movement within the CVD reactor using numerical methods. CFD models simulate the fluid dynamics, temperature distribution, and concentration profiles within the reactor, providing detailed information about the process. These models can incorporate complex geometries, boundary conditions, and reaction kinetics to accurately predict deposition behaviour (Haddadi et al., 2017; Yu et al., 2016).

5. **Multiscale models:** Multiscale models combine different modelling approaches to capture the various length and time scales involved in CVD. They integrate macroscopic models, such as CFD models, with microscopic or atomistic models to bridge the gap between the reactor-scale phenomena and the molecular-scale processes occurring at the surface. Multiscale modelling allows for a more comprehensive understanding of the CVD process and its underlying mechanisms (Kalisch et al., 2023; Ogawa et al., 2023; Yu et al., 2016).

The choice of parametric modelling approach depends on the specific objectives of the study, available data, level of understanding of the process, and computational resources. Often, a combination of different modelling approaches is used to gain a more complete understanding of the CVD process and optimize the desired outcomes. However, the development of chemical kinetics in CVD has been a crucial aspect of understanding and optimizing thin film deposition processes. CVD is a complex process that involves chemical reactions occurring at the gas-solid interface. The development of chemical kinetics in CVD is essential for understanding and controlling the deposition process, as it provides insights into the reaction mechanisms, rate-limiting steps, and the influence of process parameters on the growth of thin films or coatings. Chemical kinetics in CVD may be traced back to the mid-twentieth century when researchers began examining the gas phase and surface reactions involved in film deposition. Initially, basic empirical models based on experimental data were employed to represent the overall deposition rate (Pierson, 1999; Sun et al., 2021). However, as CVD technology advanced, more sophisticated approaches were developed to model the reaction kinetics and provide mechanistic insights. The development of chemical kinetics in CVD can be summarized as follows:

1. **Gas-phase reactions**: The initial step in developing chemical kinetics in CVD is to investigate precursor gas-phase processes. Understanding the breakdown, dissociation, and generation of reactive species from precursor molecules is part of this. Temperature, pressure, and gas composition all have an impact on gas-phase processes.

2. **Surface reactions:** Once the reactive species are formed in the gas phase, they adsorb onto the substrate surface and undergo surface reactions. These reactions involve the breaking of chemical bonds and the rearrangement of atoms on the substrate surface. Surface reactions are critical in determining the growth rate and properties of the deposited film

   Developing detailed reaction mechanisms is essential to gain a comprehensive understanding of the CVD process. This involves identifying the elementary steps involved in both gas-phase and surface reactions and determining their kinetics. Obtaining accurate rate constants for the elementary reactions is crucial for predicting the deposition rate and optimizing the CVD process. Experimental techniques, such as temperature-programmed reaction (TPR) and isothermal reaction studies, are used to measure rate constants. With the advancement of computational tools, quantum

chemical calculations and molecular dynamics simulations are employed to gain insights into the reaction mechanisms and kinetics (Benzinger et al., 1996; Hu and Hüttinger, 2001). These computational methods complement experimental studies and provide a deeper understanding of complex reactions. As CVD processes become more complex, multi-scale modelling approaches, such as Kinetic Monte Carlo simulations and continuum models, are used to bridge the gap between atomistic and macroscopic scales (Raciti et al., 2023). These models help predict film growth under various process conditions. The development of chemical kinetics in CVD continues to evolve as new materials and advanced deposition techniques are introduced. Understanding the underlying chemistry is crucial for tailoring material properties, enhancing film uniformity, and minimizing defects. It also enables the rational design and optimization of CVD processes for a wide range of applications, including semiconductor manufacturing, coating technologies, and the production of advanced materials.

2.3 Literature based on pyrolysis of methane in CVD reactor

Bourrat et al., 2006 provide a review of the current state of research on pyrocarbons produced at low temperatures (Bourrat et al., 2006b). Pyrocarbons are carbon-based materials that are produced by the pyrolysis of hydrocarbons or other organic materials. They discuss the different methods for producing pyrocarbons at low temperatures, as well as their properties and potential applications. The authors concluded that low-temperature pyrocarbons have the potential to be used in a wide range of applications, including as adsorbents, catalysts, and energy storage and conversion (Bourrat et al., 2006b).

Beigi-Boroujeni et al. (2020) describe a method for producing pyrolytic carbon from Novolac epoxy resin (Beigi-Boroujeni et al., 2019) The method involves compressing the resin before undergoing photocrosslinking and pyrolysis. They found that the compression of the resin before the pyrolysis process led to a higher yield of pyrolytic carbon, as well as improved mechanical properties. The pyrolytic carbon produced has a high specific surface area, strong electrical conductivity, and mechanical characteristics. According to their findings, this approach can be utilised to generate high-quality pyrolytic carbon from Novolac epoxy resin (Beigi-Boroujeni et al., 2020).

Tan et al. (2016) describe a method for producing large-sized, high-density, bulk isotropic pyrocarbon materials using fixed-bed CVD (Tan et al., 2016). They found that by using a

special composite microstructure, they were able to produce pyrocarbon materials with high density, good isotropy, and large size. The resulting pyrocarbon materials were found to have excellent mechanical and electrical properties, including high hardness and high electrical conductivity. The study suggests that this method is a promising approach for the large-scale production of high-quality pyrocarbon materials (Tan et al., 2016).

Chen et al. (2018) explain the use of CVD to create three-dimensional graphene materials for energy-related applications (Chen et al., 2018). The authors discuss recent advances in the CVD growth of 3D graphene materials, including distinct CVD growth methods, the synthesis of various 3D graphene structures, and the characteristics of the resulting materials. They also examine the potential applications of 3D graphene materials in energy-related disciplines such as energy storage and conversion, as well as their scalability and constraints. According to their findings, the CVD development of 3D graphene materials is a potential strategy for generating high-quality graphene materials for energy-related applications that can be scaled up for industrial production (Chen et al., 2018).

Kadinski et al. (2004) offer a computational investigation of the formation of GaN/InGaN layers in a vertical rotating disc reactor employing metal-organic chemical vapour deposition (MOCVD). The authors studied the gas flow and temperature distribution in the reactor, as well as the impact of reactor design and operating parameters on the formation of the GaN/InGaN layers, using CFD models. They discovered that the reactor design and operating circumstances have a substantial impact on the formation of the GaN/InGaN layers and that a high disc rotation rate resulted in better growth uniformity and fewer flaws. According to the findings, computational analysis can be utilised to optimise the growth of GaN/InGaN layers in MOCVD vertical rotating disc reactors, resulting in high-quality and uniform layers.

Liu et al. (2007) offer a study on the development of zinc oxide (ZnO) films using MOCVD. The authors explore the influence of growth parameters such as temperature, pressure, and precursor flow rate on the characteristics of ZnO films using a kinetic model. They discover that the film's growth rate is sensitive to these factors and that the films have good crystalline quality. According to the paper, the MOCVD method is a promising technology for the growth of ZnO films, and the kinetic model created in the study can be utilised to optimise the growth parameters for high-quality ZnO films (Liu et al., 2007).

Cheng and Hsiao (2008) report on numerical studies of the influence of geometric factors on the flow and temperature fields in a horizontal CVD reactor. CFD simulations were utilised in the study to examine the impact of various geometric characteristics, such as the reactor's aspect ratio and the position of the inlet, on the flow and temperature fields within the reactor. The

simulation findings revealed that the reactor's aspect ratio had a substantial effect on the flow and thermal fields, with larger aspect ratios resulting in more uniform flow and thermal fields. Furthermore, the position of the inlet had a considerable effect on the flow and thermal fields, with inlets situated closer to the centre of the reactor resulting in more uniform flow and thermal fields.

Wang et al. (2016) provide a study on the simulation optimisation of filament parameters for uniform diamond film deposition on surfaces of ultra-large circular holes using a CVD technique (Wang et al., 2016). The researchers performed numerical simulations to investigate the effects of various filament parameters on the uniformity of diamond film deposition, such as the distance between the filament and the hole surface, the filament diameter, and the filament shape. Based on the simulation results, the authors also offered an optimisation technique. The simulation findings revealed that the filament distance, diameter, and shape all had a substantial impact on the regularity of diamond film deposition. Overall, the work demonstrates that utilising simulation to optimise filament parameters might improve the uniformity of diamond film depositions on ultra-large circular holes using a CVD technique (Wang et al., 2016).

Barbosa et al. (2009) studied the effect of substrate temperature on the generation of ultra-nanocrystalline diamond (UNCD) films deposited using a hot filament CVD technique with an argon-rich gas mixture. The findings revealed that increasing the substrate temperature reduced the average grain size of the UNCD films while improving their crystallinity. The ideal substrate temperature for generating high-quality UNCD films, according to the authors, was around 800°C. Furthermore, Barbosa et al. (2009) discovered that UNCD films generated at higher substrate temperatures exhibited superior mechanical characteristics and increased surface roughness.

Barua and Povitsky 2020 presented a computational model for carbon CVD at internal surfaces. The model is built around a set of differential equations that characterise the mass and energy balance of the CVD process while accounting for mass transfer, heat transfer, and chemical reactions (Barua and Povitsky, 2020). The authors utilised the model to simulate the formation of carbon films on interior surfaces under various conditions and discovered that it can predict the rate of growth as well as the microstructure of the films. The work also demonstrates that the model may be used to optimise CVD process parameters like as temperature, reactant gas flow rate, and pressure to obtain desired film qualities. According to the findings, the model can be used to better understand and manage the CVD process on internal surfaces (Barua and Povitsky, 2020).

Teixeira et al., 2020 propose a CFD-based sensitivity study of the CVD process for the synthesis of carbon nanotubes (CNTs). The scientists conducted CFD simulations to study the effects of numerous process parameters on CNT growth, including temperature, reactant gas flow rate, and pressure. The temperature and flow rate of the reactant gases were shown to have a substantial influence on the formation of CNTs, while pressure had a comparatively modest effect. The results also showed that the rate of CNTs growth increased with increasing temperature and decreasing flow rate of reactant gases. According to the study, CFD simulation can be a useful tool for understanding and optimising the CVD process for CNT synthesis (Teixeira et al., 2020).

Coso et al. (2008) offer a CVD model for polysilicon development in trichlorosilane (TCS) and hydrogen environments. The authors created a set of mathematical equations to represent the mass and energy balance of the CVD process while accounting for mass transfer, heat transfer, and chemical interactions. They discovered that the rate of polysilicon growth is affected by TCS and hydrogen flow rates, substrate temperature, and pressure. They also discovered that the TCS/H_2 ratio affects polysilicon film quality and that the ideal ratio is around 1.5. Del Coso et al. (2008) found that the model can be used to estimate the growth rate and quality of polysilicon films, as well as to optimise CVD process parameters.

Lin et al., 2009 offer a parametric model for the CVD process. The model predicts the growth rate of the deposited film by taking into account several process parameters such as pressure, temperature, and reactant flow rate. This model is then used by the authors to optimise the CVD procedure for maximum growth rate (Lin et al., 2009a).

An et al. (2018) provide research on the use of response surface methodology (RSM) to optimise operating parameters in a polysilicon CVD reactor. The authors look into how process parameters like pressure, temperature, and flow rate affect the growth rate and quality of the deposited polysilicon film. RSM is used to identify the optimal operating conditions for the CVD process by analysing the relationship between process parameters and responses. The optimal working conditions for the maximum growth rate and best quality of the polysilicon film were discovered to be at a pressure of 600 Pa, a temperature of 673 K, and a flow rate of 100 sccm (An et al., 2018).

Ramadan and Im (2019b) report research on the optimisation of operational parameters in a planetary CVD reactor using response surface methodology (RSM). The authors look at how process parameters like rotation speed, substrate temperature, and flow rate affect the growth rate of the formed silicon layer. RSM is used to identify the optimal operating conditions for the CVD process by analysing the relationship between process parameters and responses. The

study discovered that the ideal working conditions for the maximum growth rate are 30 rpm rotation, 953 K substrate temperature, and 800 sccm flow rate (Ramadan and Im, 2019b).

Cheng and Hasiao (2008) study the effect of various geometric designs on the flow and temperature fields in a horizontal CVD reactor. The study uses numerical simulations to evaluate how changes in the geometric parameters of the reactor, such as its width and height, affect the distribution of reactants and the temperature within the reactor. The width and height of the reactor were discovered to have a substantial impact on the flow and temperature fields within the reactor. The study discovered that increasing the width of the reactor increases flow velocity while decreasing the height of the reactor decreases the temperature gradient. The study also discovered that the flow and thermal fields are not symmetric about the reactor's centre and that the thermal field is more sensitive to changes in the geometric parameters of the reactor than the flow field.

2.4 Use of machine learning (ML) in chemical processes

Jia et al. (2017) offer a study that combines the usage of a Support Vector Machine (SVM) and Particle Swarm Optimisation (PSO) to optimise the design of a dividing wall column (DWC) for binary mixture separation (Jia et al., 2017a). SVM was used to predict the link between the DWC design parameters and separation performance, and PSO was used to find the ideal set of design parameters that maximised separation efficiency. The study's findings revealed that the SVM-PSO strategy was capable of effectively optimising the DWC design and improving separation efficiency (Jia et al., 2017a).

Wu et al., 2020 present the development of a new computational algorithm called Inverse Quantitative Structure-Property Relationship (IQSPR) implemented in the open-source platform XenonPy (Wu et al., 2020b). The IQSPR algorithm uses Bayesian Machine Learning to predict the structural and electronic properties of a molecule from its experimental thermodynamic data, such as boiling point, melting point and heat of vaporization. The authors tested the performance of IQSPR using a dataset of organic compounds and reported a high accuracy in the predictions (Wu et al., 2020b)**.**

Masoumi et al. (2014) propose a study that used a wavelet neural network (WNN) to optimise the process parameters for the lipase-catalyzed production of ester amines-based esterquats in a 2-liter bioreactor. WNN was utilised by the authors to simulate the link between process factors (such as temperature, pH, and substrate concentration) and the esterquat conversion

rate. The WNN model was then utilised to optimise the process parameters to get the highest conversion rate possible. The study's findings revealed that the WNN model could properly forecast the esterquat conversion rate and that optimising the process parameters increased the conversion rate (Fard Masoumi et al., 2014).

Chuang and Chen (2014) offer a mathematical model of a MOCVD reactor for gas film growth. They use this model to improve the growth of the films by optimising the reactor architecture. They also present a method for adjusting the reactor's temperature to achieve optimal growth conditions. According to the findings of the study, the proposed model and design can improve the efficiency of the MOCVD process for gas film growth (Chuang and Chen, 2014).

Azarpour et al. (2017) provide a generic hybrid model for the analysis of industrial fixed-bed catalytic reactors. To anticipate reactor performance, the approach integrates mathematical modelling, artificial neural networks, and experimental data. The model was applied to a variety of fixed-bed catalytic reactors, including those used to produce hydrogen, methanol, and ethylene. The model was found to be capable of properly predicting reactor performance, including conversion and selectivity of the catalytic reaction. The authors also discovered that the model might be used to optimise the reactor's operating settings to increase its performance (Azarpour et al., 2017).

Yang et al. 2020 describe a hybrid model for predicting fluid catalytic cracking performance that incorporates deep learning and mechanistic kinetics. The scientists used experimental data to develop a deep learning model, which they then used to predict the performance of a fluid catalytic cracking reactor. They combined the deep learning network's predictions with a mechanistic kinetics model to boost prediction accuracy. The hybrid model effectively predicted the performance of the fluid catalytic cracking reactor, including conversion and product distribution, according to the scientists. They also discovered that the hybrid model outperformed other models based only on deep learning or mechanistic kinetics (Yang et al., 2020).

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