Analysis of the Two-dimensional Material Preparation Process Based on CVD TECHNOLOGY

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Abstract. The extensive discovery of two-dimensional materials has promoted the development of manufacturing technologies for two-dimensional thin films. Although CVD technology has been widely applied in the production of large-sized two-dimensional thin films, there is still room for improvement in the manufacturing of high-quality large-sized two-dimensional thin films. This paper discusses the process and basic principles of CVD technology in the manufacturing of two-dimensional materials, common optimization methods, and prospects for future optimization directions. Firstly, it introduces the gas-phase transformation of reactants, gas-phase reaction of reactants, transport of reactants, reactions on the substrate, and the final emission of reaction products in CVD technology. Then, it presents common optimization schemes for CVD technology, including low-pressure chemical vapor deposition, plasma-assisted chemical vapor deposition, and laser chemical vapor deposition. Through a comparative analysis of existing optimization techniques, it is concluded that effective optimization may be achieved in the gas-phase transformation of reactants and the deposition process in the future, providing a useful reference for the development and application of CVD technology.

Keywords: Chemical vapor deposition; Thin film material; Gas-phase conversion; Vapor deposition.

1. Introduction

Since graphene was discovered in 2004, the preparation and application of two-dimensional materials have received extensive attention and research [1]. Two-dimensional transition metal chalcogenide materials (TMDs) are a new type of material, featuring atomic-level thickness and periodic arrangement [2]. This structure endows TMDs with excellent physical, chemical and mechanical properties [3], making them one of the most promising semiconductor materials for continuing Moore's Law of integrated circuits in the post-Moore era [4]. The main methods for preparing TMDs at present include micromechanical exfoliation [5], molecular beam epitaxy (MBE), and chemical vapor deposition (CVD) [6].

2. The Basic Principles and Process of CVD Technology

The principle of CVD is to place the reaction substrate in a gaseous reaction medium, allowing the reactants to undergo chemical reactions on the substrate surface and form a solid film on the substrate. The process of CVD takes place in a reaction gas-phase deposition system. Firstly, the high-purity solid reaction precursors are evaporated in the vaporization zone and the gaseous precursors are transported to the reaction zone through an inert carrier gas. Secondly, on the substrate surface, the gaseous precursors react and release active molecules, which deposit on the substrate surface. Meanwhile, the by-products generated during the reaction are removed by the vacuum pump system.

2.1. The vaporization of reactants

Different reactants have different vaporization temperatures and vaporization conditions. For solid or liquid reactants with high vapor pressure, the reaction can be vaporized by direct heating and evaporation [7]. For liquid reactants with low vapor pressure, the bubble method can be used. The carrier gas is introduced into the liquid reactant to vaporize the reactant and mix it in the carrier gas [7]. For solid reactants with high sublimation temperatures, the laser ablation method can be used.

High-energy laser beams are used to directly vaporize the material, as shown in Figure 1. However, this method has the disadvantage of high cost [8].

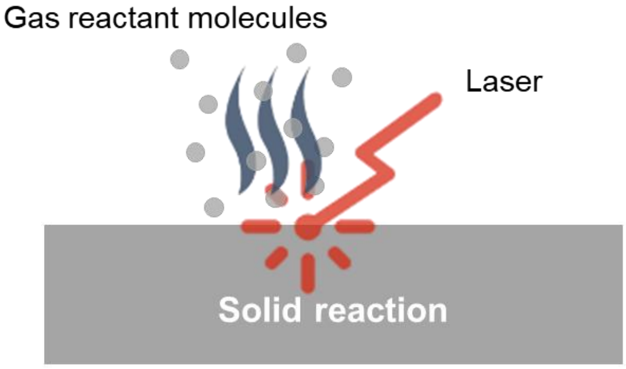

Figure.1 Using high-energy laser to vaporize soild reactants

During the gasification process of the reactants, it is necessary to control the gasification temperature, gasification pressure, carrier gas type, and the timing of adding the reactants. Controlling the gasification temperature can regulate the concentration of gaseous reactants, but excessively high temperatures may cause the reactants to decompose. The gasification pressure has a certain influence on the gasification of the reactants. Lower pressure is conducive to the gasification of the reactants, but too low pressure may lead to uneven subsequent reaction processes. The carrier gas is usually selected as an inert gas to avoid reacting with the reactants. The flow rate of the carrier gas is also an important factor in controlling the gas-phase deposition reaction. An excessive carrier gas flow rate will result in uneven deposition reactions. The timing of adding the reactants will also affect the gasification process. Different reactants have different gasification temperatures, so the heating time varies, and it is necessary to reasonably arrange the heating time for different components to ensure that the gaseous reactants have sufficient concentration when reaching the deposition temperature [9].

2.2. Reaction of Gaseous Reactants

After the reactants are vaporized, the generated gaseous reactants diffuse and mix within the carrier gas, and then undergo a chemical reaction in the reaction chamber to produce the precursors of the film-forming substances. For example, in a CVD system using silane (SiH4), silane will decompose in the gas phase, generating intermediate products such as SiH3 and SiH2 [8]. In the metal organic chemical vapor deposition method, the precursor vapor undergoes thermal decomposition, generating reactants used for film formation [10].

However, if the gaseous reactants react in areas outside the substrate surface, it may have a negative impact on the formation of the film. For example, when using S and MO3 as solid reactants for the vaporization process, the sequence of reactant vaporization needs to be controlled. If the sulfur source starts to vaporize earlier than MO3, it will cause the MO3 to undergo sulfidation, resulting in contamination and reducing the concentration of reactants released by the molybdenum source [9]. By controlling the time difference between the start of heating of the reactants, both can reach the vaporization temperature simultaneously.

2.3. Transport of Gaseous Reactants to the Substrate

The transportation of gaseous reactants under normal pressure conditions usually employs carrier gas and relies on fluid transportation and diffusion as the means of transport. There are also cases where, under low pressure or even in a highly vacuum environment, the transportation of gaseous reactants is achieved by utilizing the principles of molecular dynamics.

Before the gaseous reactants are transferred to the substrate, it is necessary to remove the existing gases in the reaction chamber. Usually, an air pump is used to evacuate the reaction chamber to a vacuum state and remove the air inside. Then, a carrier gas is introduced to the target pressure and maintained for a period of time to fill the reaction chamber with the carrier gas. The carrier gas should generally not react with the gaseous reactants and is usually selected from hydrogen, nitrogen or inert gases.

In APCVD, the transport mode of the gaseous reactants follows the diffusion and convection mechanisms of gases and is subject to the influence of the concentration gradient of the reactants and the flow of the carrier gas, resulting in directional transfer. In LPCVD, the diffusion effect of the reactant molecules becomes the main transfer mechanism, causing the reactant molecules to transfer from high concentration to low concentration.

2.4. The Reactants Undergo Reactions on the Surface of the Substrate

In CVD technology, common substrate materials include metallic and alloy substrates such as copper substrates and Cu-Si alloy substrates, semiconductor substrates such as single-crystal silicon wafers and single-crystal germanium wafers, and insulating substrates such as quartz and sapphire substrates [11]. The crystal structure of the substrate has a significant impact on the crystal quality and orientation of the film formed by the reactant deposition [12]. Therefore, when depositing films, it is necessary to select a suitable substrate crystal structure that matches the crystal structure of the film.

The physical properties of the substrate material also need to be given special consideration. When the thermal expansion coefficients of the substrate and the film differ significantly, during the cooling process, the release of stress can easily cause the film to develop wrinkles, thereby reducing the quality of the film [12]. If the reactant atoms have a high solubility in the substrate and a low diffusion rate, it will also have a certain impact on the uniformity of the film [12].

2.5. Excretion of By-products after the Reaction

After the gaseous reactants react on the substrate surface, some of the reactions will produce by-products, which need to be promptly removed from the reaction chamber. Generally, a vacuum pump is used and a carrier gas is continuously introduced to carry the by-products from the reaction area to the exhaust port, achieving the removal of the reaction products [13]. In addition, the geometric shape of the reaction chamber will affect the flow pattern of the carrier gas. Reasonable design of the gas flow pattern within the chamber is helpful to improve the efficiency of removing the reaction products [13].

3. Common Optimization Schemes for CVD Technology

3.1. Low-pressure Chemical Vapor Deposition (LPCVD)

LACVD is a chemical vapor deposition process carried out under low-pressure conditions. It has the advantages of uniform film deposition, low particle contamination, and high deposition efficiency. Moreover, in complex device structures, LPCVD exhibits excellent step coverage and can grow uniformly in both vertical and horizontal directions.

In practical applications, for some two-dimensional materials such as graphene and GaSb, if grown using APCVD, there may be difficulties in growth or poor growth quality [14]. The reason is that at normal pressure, the nucleation density during the deposition of two-dimensional materials is relatively high, which will lead to a reduction in the size of the grown crystal domains. The different crystal orientations between each crystal domain, it affects the neatness and uniformity of the material [15].

To address these issues, the low-pressure chemical vapor deposition method can be adopted. This method can effectively reduce the nucleation density during material growth, which is beneficial for the growth of large crystal domains. Subsequently, through annealing treatment, the cleanliness and quality of the deposited film can be further optimized. Xu et al. found that after annealing the Zn:O film prepared by LACVD, the defects at the grain boundaries were effectively repaired, and the electrical properties of the film were improved [16].

3.2. Plasma-assisted chemical vapor deposition (PECVD)

PECVD generates plasma through the excitation of microwaves or electric currents. The high-energy electrons in the plasma can ionize the reactants, thereby producing a large number of reactive radicals and ions [17]. These chemically active groups then diffuse onto the substrate surface and deposit to form a film.

The advantage of this method lies in the use of high-energy electrons in the plasma to vaporize the reactants, which is different from the traditional thermal decomposition method. It does not require a high vaporization temperature and also reduces the requirement for the substrate temperature. Therefore, this technology is applicable to a wider range of substrates and film materials, such as depositing SiOx films on flexible polyester films [18]. Moreover, the large amount of active reactants in the plasma enables this method to have a higher deposition rate.

3.3. Laser Chemical Vapor Deposition (LCVD)

In LCVD, the dissociation of reactant molecules occurs through two mechanisms: the photolysis mechanism and the photodissociation mechanism [19]. The photolysis mechanism is similar to the traditional CVD technology mechanism, where the reactant molecules are dissociated by the heat field, generating a large number of active molecules for the deposition reaction. Compared with traditional CVD technology, LCVD can form a more controllable thermal field, has stronger selectivity for the deposition area, and is suitable for the deposition process of fine device structures.

The photolysis mechanism involves the use of high-energy photons to break the chemical bonds of reactant molecules, resulting in the formation of active molecules. These active molecules then adsorb and deposit on the substrate surface, forming a film. The advantage of this method lies in the fact that by applying lasers with specific wavelengths and powers to the precursors, it effectively reduces the temperature conditions required for deposition during the photolysis process and lowers the stress required for film formation [19]. However, its limitation is that during the photolysis process, molecular clusters are prone to form, and the deposition of these clusters on the substrate surface may lead to contamination of the film [20].

3.4. Metal Organic Chemical Vapor Deposition (MOCVD)

MOCVD also achieves the preparation of thin films through gas-phase reactions. This technology uses metal-organic compounds as the precursors for the reaction, causing them to decompose on the substrate surface and release metal atoms and other elements. Subsequently, these active metal atoms react on the substrate surface, eventually forming a film material with better uniformity [21].

The metal-organic chemical vapor deposition method has the advantage of controllable reaction rate. Since the reaction precursors are generally introduced in the form of gases, the reaction rate can be controlled by adjusting factors such as gas flow rate, gas pressure, and reaction temperature. Moreover, the metal-organic vapor deposition method can be carried out at a lower pressure, which can improve the uniformity and purity of the formed films. At the same time, the metal-organic chemical vapor deposition method has the advantage of a wide range of applicable materials, and can be used for the growth of metal, semiconductor, and oxide film materials.

4. Prospects for the Optimization of CVD Technology

With the development of CVD technology, the optimization approach for future technologies can start from aspects such as the deposition environment, substrate material, deposition film material, and deposition technique, and be carried out with targeted optimization in accordance with actual process requirements.

In terms of the deposition environment, CVD technology is not limited to being carried out under normal pressure conditions. Conducting chemical vapor deposition under low pressure not only reduces the nucleation density of the deposition, increases the size of the crystal domains, but also improves the quality and uniformity of the deposited film. For film materials that are difficult to grow or have poor quality under normal pressure, conducting chemical vapor deposition under low pressure can effectively enhance the film formation quality. In the future, the optimization of the deposition environment may involve conducting chemical vapor deposition under high vacuum conditions, further reducing the nucleation density of the deposition and improving the uniformity and quality of the deposited film.

The selection of substrate materials has become more diverse in accordance with the requirements of the research scenarios. From metallic and alloy substrates, to semiconductor and its oxide substrates, and then to polyester-based flexible material substrates. When the deposited film crystal structure is similar to that of the substrate, it usually improves the growth quality of the film. For hard substrate materials, in the future, the surface of the substrate can be optimized to improve the flatness and thermal strain performance of the substrate surface, and optimize the connection mode between the film and the substrate during the deposition process. While growing film materials on flexible material substrates, in the future, it may play a role in the field of flexible electronic circuits.

In the field of deposited thin film materials, the scope has expanded from elemental materials such as graphene and silicon semiconductors to other compound materials such as transition metal chalcogenides. In the future, more complex material systems' thin films can be fabricated through CVD, such as wide-bandgap semiconductors composed of multiple elements, or more complex thin film devices.

In terms of the vaporization of reactants and pre-treatment, methods such as using laser evaporation of reactants or forming precursor vapors by combining organic substances with reactants have been employed. These methods can reduce the temperature required for evaporation to a certain extent. In the future, by optimizing the vaporization method of reactants and pre-making the reactants into nanoscale particles, the temperature conditions required for reactant vaporization can be further reduced; high-energy lasers can also be used to quantitatively control the mass of vaporized reactants, reducing the waste of reactant materials; or new metal organic precursor materials can be developed to reduce the generation of by-products during decomposition and improve the purity of the formed films.

Currently, CVD technology has been widely applied in manufacturing the metal tungsten thin layer for device gate contacts and TMDs film materials. However, there are still certain difficulties in regulating the growth parameters and achieving high-quality uniformity of the films. In the future, different optimization schemes of CVD technology, or combined with other physical and mechanical methods, can be used to improve the above problems and enhance the selectivity and quality during the film growth process.

5. Conclusion

CVD technology has become an important means for manufacturing two-dimensional thin film materials and has attracted extensive research. This paper systematically elaborates on the basic process and principles of the chemical vapor deposition method, and summarizes and analyzes its common optimization schemes. In current research, most optimization schemes focus on the gas-phase conversion of reactants and the gas-phase deposition process. It is believed that with the advancement and development of CVD technology, the gas-phase conversion and deposition processes will be further optimized, thereby improving the gasification efficiency of reactants, accelerating the film formation speed, and optimizing the film quality. This will provide reliable and efficient solutions for the development and iteration of integrated circuits, especially for specific device manufacturing processes.

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