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Research and Analysis on Semiconductor Material Manufacturing Technology

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Abstract:

Chemical vapor deposition (CVD) technology, as one of the core processes in semiconductor manufacturing, plays an irreplaceable role in modern integrated circuit production. This report systematically reviews research advances in CVD process parameter optimization, novel metal-organic precursors development, atomic-scale CVD modeling, and machine-learning-assisted optimization methods. By delving deeply into the optimization strategies of CVD process parameters, the latest understanding of reaction mechanisms, and the development progress of new precursors, the key challenges and future development directions faced by this technology are revealed. Research shows that CVD technology has made significant breakthroughs in achieving atomic-level thickness control, three-dimensional structure coverage, and low-temperature deposition, providing important technical support for the manufacturing of advanced semiconductor devices. Through systematic comparison of different CVD variants and their applicability in next-generation semiconductor devices, this review provides specific insights into future technological developments, particularly in the areas of atomic-scale precision control and three-dimensional integration.

Keywords: Chemical vapor deposition, Process optimization, Precursor design, Atomic layer deposition.

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1. Introduction

As semiconductor technology continues to evolve toward smaller feature sizes and higher integration densities, manufacturing precision requirements are approaching physical limits. At 3-nanometer and more advanced technology nodes, the challenge involves achieving atomic-level precision in material deposition with minimal margin for error [1].

The development of CVD technology spans several decades, evolving from basic thermal deposition processes to sophisticated techniques capable of atomic-scale control. Current research primarily focuses on three main technical approaches: thermal activation methods, plasma-enhanced processes, and atomic layer deposition techniques. Compared to existing reviews that often concentrate on individual aspects of CVD technology, this study provides a comprehensive analytical framework that integrates fundamental mechanisms, process optimization strategies, and emerging innovation pathways. Smith et al. demonstrated that even advanced CVD processes exhibit film non-uniformity causing approximately 5% performance variation, which becomes unacceptable at 3-nanometer technology nodes. Kim et al. revealed through in-situ characterization that when feature sizes shrink below 10 nanometers, fundamental changes in surface reaction kinetics render traditional process windows ineffective [2]. This explains why empirical optimization methods show limited effectiveness in next-generation device manufacturing.

Current research gaps persist in understanding precursor-surface interactions at atomic scales [3], establishing quantitative models for coupled transport-reaction mechanisms in multi-physics environments, and developing suitable process solutions for novel device structures like GAA transistors.

This paper analyzes the applicability of different CVD variants in advanced device manufacturing, explores machine learning-based optimization methods [4], and systematically evaluates application prospects of various CVD processes in semiconductor manufacturing.

2. Theoretical Basis Analysis

2.1 Basic Principles and Reaction Mechanisms of Chemical Vapor Deposition Technology

The essence of chemical vapor deposition is the process in which gaseous precursors undergo chemical reactions on the surface of a heated substrate to form solid films. This process involves multiple steps such as complex gas-phase reactions, surface adsorption, chemical reactions and desorption of by-products. The driving force of the CVD process comes from the reduction of the system‘s free energy, and the deposition rate is jointly controlled by mass transfer, surface reaction and nucleation process. Recent studies have found that at the nanoscale, the surface reaction mechanism undergoes significant changes. The simulation study by Johnson et al. shows that the traditional Langmuir-Hinshelwood mechanism gradually gives way to the Eley-Rideal mechanism, which changes the dependence of the reaction rate on temperature and partial pressure of the precursor.

2.2 Characteristics and Application Scope of CVD Technology

Atmospheric Pressure CVD (APCVD) operates under ambient pressure conditions, featuring relatively simple equipment configurations and high deposition rates typically reaching 100-500 nm/min. However, limitations in reactive gas diffusion under atmospheric conditions result in poor film uniformity (>10% non-uniformity) and restricted step coverage capability. This technology primarily serves applications requiring thick films where superior uniformity is not critical, such as buffer or protective layers, with limited utilization in advanced-node semiconductor manufacturing [5].

Low-Pressure CVD (LPCVD) conducts deposition under reduced pressure conditions (13.3-1330 Pa), characterized by exceptional film uniformity (<5% non-uniformity) and excellent step coverage capability. The requirement for high processing temperatures (>600°C) restricts application in thermally sensitive materials. LPCVD finds extensive use in depositing critical films including polysilicon and silicon nitride, playing vital roles in semiconductor device fabrication, particularly in gate formation and isolation layer processes [6].

Plasma-Enhanced CVD (PECVD) utilizes plasma activation of chemical reactions, significantly reducing deposition temperatures to below 300°C while maintaining high-quality film formation. This characteristic makes it particularly suitable for temperature-sensitive back-end processes, though plasma introduction may cause plasma-induced damage requiring precise parameter control. PECVD primarily applies to dielectric layer deposition such as passivation and insulation layers, maintaining crucial importance in modern integrated circuit manufacturing [7].

Atomic Layer Deposition (ALD) employs self-limiting surface reactions through alternating precursor introduction to achieve atomic-level thickness control. This technology provides exceptional film uniformity (<2% non-uniformity) and superior three-dimensional structure coverage capability. The unique deposition mechanism results in relatively low deposition rates (1-10 nm/min). ALD proves particularly suitable for applications demanding extreme thickness and uniformity control, including high-k dielectric layers and diffusion barriers, gaining increasing prominence in advanced semiconductor device manufacturing [8].

3. Quantitative Analysis and Performance Comparison

3.1 Performance Characteristics Analysis of Different CVD Technologies

Statistical analysis of various CVD techniques reveals significant differences in deposition characteristics. Atomic layer deposition demonstrates the broadest temperature adaptability (150-350°C), while low-pressure CVD requires substantially higher processing temperatures (550-650°C) [6,8]. Atmospheric pressure CVD shows distinct advantages in deposition rate (100-500 nm/min), whereas ALD technology maintains considerably lower rates (1-10 nm/min) [5,8]. Film uniformity analysis indicates ALD achieves superior performance (1-2% non-uniformity), contrasting with APCVD's relatively higher non-uniformity (8-15%) [5,8]. ALD technology exhibits exceptional three-dimensional structure coverage, while APCVD demonstrates limited capability in this aspect [5,8]. These performance differences determine their respective applicability conditions, with ALD being preferred for high-precision applications and APCVD remaining suitable for less demanding thick-film applications.

3.2 Research Progress on the Influence of Process Parameters

In temperature effects research, Zhang et al. systematically investigated deposition temperature impacts on SiO2 film stress using design of experiments methodology [10]. Their results demonstrate temperature's predominant influence on film stress, with compressive stress increasing approximately 200 MPa per 50°C temperature increment. This finding provides crucial theoretical foundation for film stress optimization in advanced semiconductor devices.

In pressure parameter optimization, Thompson's team employed computational fluid dynamics to simulate pressure variation effects on film uniformity [11]. Their simulations reveal significant changes in reactive gas flow states and boundary layer thickness within 13.3-133 Pa range, directly affecting deposition uniformity. Through pressure parameter optimization, film non-uniformity can be reduced over 40% within the optimal 40-60 Pa window .

Regarding precursor flow rate effects, Wilson et al. experimentally examined relationships between precursor flow rate and deposition rate [12]. Their research indicates linear positive correlation between deposition rate and flow rate under constant precursor concentration conditions. However, beyond certain critical flow rates, further increases produce diminishing returns on deposition rate enhancement and may compromise film quality.

4. Key technical Challenges and Innovation directions

4.1 Main Technical Challenges Faced by the Manufacturing Process

In terms of atomic-level precision control, since the feature size of semiconductor devices continues to shrink to the technical node below 3 nanometers, the control requirements for film thickness and composition have reached the atomic level. The existing CVD technology still faces severe challenges in achieving sub-angs-level thickness control in large-scale production. Specifically, when the thickness of the film is controlled at the scale of a few atomic layers, traditional thickness monitoring methods are difficult to meet the accuracy requirements, and at the same time, the impact of process fluctuations on the performance of the film is significantly magnified. Furthermore, at the atomic scale, the adsorption and dissociation behaviors of precursor molecules exhibit characteristics that are completely different from those at the macroscopic scale, which requires us to have a deeper understanding of the surface reaction mechanism. To address this challenge, it is essential to develop new in-situ monitoring technologies and more precise process control methods [13].

In terms of three-dimensional structure coverage capability, advanced device structures such as fully surround gate (GAA) transistors require CVD technology to achieve perfect conformal deposition in nanostructures with an extremely high aspect ratio (greater than 10:1). The current step coverage capability of CVD technology is still insufficient to meet these demanding requirements. In structures with an increasing aspect ratio, the diffusion limitations of reactive gases and the differences in surface reaction probabilities can lead to an uneven distribution of film thickness, which in turn affects the consistency of device performance. Especially in the bottom and corner areas of the structure, due to insufficient supply of precursors, problems such as incomplete deposition or decline in film quality often occur. This needs to be addressed by optimizing the reactor design, improving the precursor delivery system and developing new deposition strategies [14].

In terms of the challenge of thermal budget constraints, as the complexity of semiconductor manufacturing processes continues to increase, the requirements for thermal budgets in back-end processes are becoming increasingly strict, and there is an urgent need to develop deposition processes at lower temperatures. However, reducing the deposition temperature often comes at the expense of film quality. How to obtain high-quality film materials under low-temperature conditions has become a key issue that needs to be urgently addressed. Low-temperature deposition usually leads to a series of problems such as reduced film density, increased defects, and difficult stress control, which directly affect the reliability and performance of the device. Therefore, it is necessary to explore new reaction mechanisms and activation methods to achieve true

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low-temperature deposition while maintaining the quality of the film, which is of great significance for the manufacturing of the next generation of semiconductor devices [15].

4.2 Future Technological Development Directions

In the field of new precursor design, researchers are developing precursor materials with specific reaction characteristics through precise molecular engineering design. By introducing steric hindrance groups into the molecular structure, the surface reaction kinetics can be precisely controlled, achieving better step coverage and film uniformity. Designing precursors with self-limiting reaction characteristics is another important direction. Such precursors can achieve CVD processes similar to atomic layer deposition while maintaining a relatively high deposition rate. In addition, developing a stable liquid precursor delivery system is also a research focus, which can enhance the accuracy of process control and process repeatability. These innovations will significantly enhance the applicability of CVD technology in advanced semiconductor manufacturing.

In terms of plasma-assisted technological innovation, the adoption of new plasma sources such as remote plasma and pulsed plasma shows great potential. Remote plasma technology can effectively separate the plasma region from the deposition region, significantly reducing plasma-induced damage. It is particularly suitable for the manufacturing of high-performance devices that are sensitive to defects. Pulse plasma technology can independently regulate various parameters during the thin film deposition process by precisely controlling the on and off times of the plasma, achieving better control over the characteristics of the thin film. These advanced plasma technologies not only enhance reactivity and achieve lower deposition temperatures, but also improve the microstructure and electrical properties of thin films [16].

In the field of machine learning-assisted optimization, researchers are developing intelligent process optimization systems. By building an accurate prediction model for process parameters and film properties, precise control and optimization of the deposition process can be achieved. These models can handle complex nonlinear relationships and identify the best process Windows that are difficult to discover by traditional methods. The real-time process monitoring and adjustment system based on machine learning can promptly detect process deviations and automatically correct them, significantly enhancing process stability and product yield. In addition, machine learning methods can significantly reduce the number of experiments required for process development, accelerate the research and application of new processes, and bring revolutionary progress to semiconductor manufacturing.

5. Conclusion

As a core process in semiconductor manufacturing, CVD technology is facing unprecedented challenges and opportunities. This article, through systematic analysis, indicates that: Firstly, the traditional CVD process model needs to be re-examined and revised at the nanoscale. The changes in surface reaction mechanisms require us to develop new theories and models to guide process optimization. Secondly, through innovative methods such as new precursor design, plasma-assisted technology and machine learning optimization, CVD technology is expected to break through the current technical bottlenecks and meet the strict requirements of advanced device manufacturing. Finally, the development of CVD technology needs collaborative innovation across multiple disciplines, including the deep integration of fields such as chemistry, materials science, plasma physics, and computer science. Future research should focus on atomic-level deposition mechanisms, the development of new precursors, and intelligent process control, etc., to provide technical support for the next generation of semiconductor manufacturing.

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