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Key Influences on the Preparation of Carbon Nanotubes by Chemical Vapour Deposition: Optimisation of Catalysts, Gas Parameters and Reaction Conditions

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Abstract: Carbon nanotubes (CNTs) have garnered significant interest in the field of nanomaterials due to their remarkable physicochemical properties, including exceptional strength, electrical conductivity, and thermal stability. The predominant method for synthesizing CNTs is chemical vapor deposition (CVD), a process that allows for precise control over the nanotube characteristics. This paper investigates the crucial roles of catalysts, reaction gases, and specific reaction conditions in the CVD method for CNT growth. It elaborates on how the selection of an appropriate catalyst, optimization of gas flow rates, and meticulous control of reaction temperature and duration can significantly influence the growth rate, structural integrity, and overall quality of the produced CNTs. Furthermore, the study confirms that by strategically adjusting these parameters, both the yield and purity of CNTs can be markedly enhanced. Ultimately, the objective of this paper is to provide insights that will facilitate the broader industrial application of CNTs, contributing to advancements in various fields such as electronics, materials science, and nanotechnology by optimizing the critical factors that affect their synthesis. This work aims to pave the way for innovative applications of CNTs in emerging technologies.

Keywords: Carbon nanotube, Chemical Vapour Deposition, catalyst.

1. Introduction

Carbon nanotubes (CNTs) have rapidly become a research hotspot in the field of nanomaterials due to their unique structure and excellent physicochemical properties since they were first discovered by a Japanese scientist, Sumio Iijima, through high-resolution transmission electron microscopy in 1991. Carbon nanotubes have excellent electrical, thermal and mechanical properties due to their very high aspect ratio and unique hollow structure, which have shown a wide range of applications in the fields of field-emitting materials, hydrogen storage, high-strength composites and energy storage[1].

At present, the preparation methods of carbon nanotubes mainly include are discharge method, laser ablation method and chemical vapour deposition (CVD)method. Among them, although the arc discharge method and laser ablation method can obtain high-quality carbon nanotubes, it is difficult to meet the industrial demand due to its high cost and the limitation of large-scale production. In contrast, CVD has become one of the main methods for carbon nanotube preparation due to its low equipment cost, process controllability, and suitability for large-scale production. The core principle of CVD is to decompose the carbon source gas under high temperature by the action of catalyst, and carbon atoms are deposited on the surface of the catalyst and grow carbon nanotubes gradually. However, despite the significant advantages of the CVD method, it still faces problems such as directional growth, uniformity control and crystallization defects in practical applications, which limit the large-scale application of carbon nanotubes to a certain extent.

In the CVD method. the choice of catalyst, reaction gas and reaction conditions are the key factors affecting the quality of carbon nanotube growth. The catalyst not only determines the growth rate of carbon nanotubes, but also directly affects their structure and properties; different catalyst materials and their morphologies can significantly change the diameter, length and purity of carbon nanotubes. The optimization of the reaction gas can improve the conversion efficiency of the carbon source, which further enhances the growth rate and the overall quality of carbon nanotubes, while the reaction conditions affect the deposition behavior and crystallization properties of carbon atoms[2]. Therefore, an in-depth study of these factors and their interactions is essential to optimise the carbon nanotube preparation process. Therefore, this paper will focus on the optimization of catalysts. Reaction gases and reaction conditions during the preparation of carbon nanotubes by CVD. Through in-depth analysis of the mechanism of these key factors, we hope to provide a theoretical basis and practical guidance for the preparation of high-quality carbon nanotubes, and to promote the wide application of carbon nanotubes in the industry.

2. Key influences on the preparation of carbon nanotubes in chemical vapour deposition methods

2.1. Catalysts

In chemical vapour deposition (CVD), the catalyst plays a decisive role in the growth of carbon nanotubes (CNTs), which not only affects the growth rate and yield of CNTs, but also directly determines the structure and morphology of CNTs as well as their electronic properties. The growth of single-walled carbon nanotubes (SWNTS)depends on the strong adhesion between the catalyst particles and the nanotubes, and since the strength of adhesion is closely related to the choice of catalyst materials. Catalyst materials such as iron, cobalt, nickel and so on are widely used in the synthesis of SWNTs, which is attributed to the fact that these metals can effectively catalyze the decomposition of the carbon source at high temperatures and promote the growth of carbon atoms in a helical structure, resulting in a strong carbon decomposition during the synthesis of SWNTs. synthesis process with strong carbon-metal bonding. In addition, the interaction between the catalyst and the carrier is also a key factor affecting the quality of carbon nanotube growth, which is attributed to the fact that the catalyst particles may sinter when the interaction is too weak to effectively control the growth, while too strong of an interaction will inhibit the deposition of carbon atoms[3]. Therefore, rational control of such interactions becomes an important way to prepare high-quality CNT.

Alloy catalysts can effectively control the size and distribution of catalyst particles by adjusting the ratio of metal components, which in turn affects the diameter and the number of wall layers of carbon nanotubes. The combination of Mo as a co-catalyst with iron or cobalt can dramatically increase the catalytic efficiency and improve the quality of carbon nanotube growth. Meanwhile, the size of catalyst particles also determines the diameter distribution of carbon nanotubes, with smaller catalyst particles tending to produce finer SWNTs, while larger particles tend to lead to the generation of multi-walled carbon nanotubes. This is attributed to the low curvature of the larger particles limiting the formation of SWNTs, while the high curvature of the smaller particles favours the nucleation and growth of single-walled carbon nanotubes[4]. To further improve the growth

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efficiency and structural control of CNTs, the diameter distribution of catalyst particles can be precisely controlled by adjusting the proportion of metals in the alloy to optimise the growth conditions of carbon nanotubes.

The particle size and morphology of the catalyst also affect the growth of carbon nanotubes, which is attributed to the fact that the smaller the particle size of the catalyst, the smaller the diameter of the grown CNTs and the more uniform the structure. Therefore, by precisely controlling the particle size of the catalyst, effective control of the diameter of the carbon nanotubes can be achieved, reducing the agglomeration of the catalyst particles and thus forming finer and more uniform CNTs and because the use of different metal precursors or adjusting the preparation conditions of the catalysts can further optimise the distribution of the particles and promote the growth of single-walled carbon nanotubes. And the statistical mechanics model shows that the size of catalyst particles is closely related to the nucleation state of carbon nanotubes, and larger catalyst particles tend to form multi-walled carbon nanotubes, while smaller particles are more suitable for the growth of SWNTs[5]. Therefore, the particle size and morphology of the catalyst play an important role in the growth of carbon nanotubes.

In summary, catalyst materials, particle size and their interactions play a decisive role in the synthesis of carbon nanotubes, and the application of alloy catalysts can effectively optimise the growth conditions of CNTs and enhance their quality.

2.2. Reaction gas

The type and flow rate of the reaction gas are important factors affecting the quality and properties of carbon nanotubes (CNTs)prepared by chemical vapour deposition (CVD). The selection of suitable carbon source, carrier and auxiliary gases, and the precise control of gas flow and pressure can optimise the growth process of CNTs and ultimately obtain carbon nanotubes with specific structures and properties. Carbon source gas is the main raw material for CNT growth, which is directly related to the growth rate and quality[6]. Commonly used carbon source gases, such as: hydrocarbons such as methane, ethylene and acetylene. On the one hand, gases with less carbon content can produce high-purity CNTs, which is favourable to the growth of single-walled carbon nanotubes; gases with higher carbon content usually produce multi-walled carbon nanotubes and more amorphous carbon: on the other hand, there is a significant difference in decomposition temperatures among different carbon source gases, e.g., methane, although it is more difficult to decompose, which leads toa slower growth rate, usually produces higher-quality CNTs, whereas ethylene and acetylene decompose with a higher quality, and ethylene and acetylene decompose with a lower temperature, which leads to a lower growth rate. For example, methane is easier to decompose, resulting in a slower growth rate, but usually produces higher quality carbon nanotubes, whereas the decomposition of ethylene and acetylene is easier, resulting in a faster growth rate, but may lead to non-uniformity in CNT quality. Because these differences ultimately manifest themselves in the growth rate and compositional morphology of CNTs, the appropriate carbon source gas is important for the preparation of carbon nanotubes with specific structures and properties.

Carrier gases also play a vital role in the reaction process as they transport the carbon source gas and regulate the atmosphere of the reaction. Commonly used auxiliary gases include hydrogen, nitrogen and argon. Among them, hydrogen can not only reduce the catalyst, but also etch the amorphous carbon, thus improving the purity of CNT. Argon and nitrogen, on the other hand, can protect the catalyst and carbon nanotubes from oxidation. Hydrogen, on the other hand, shows excellent etching ability, it is able to interact with the growing CNTs on the catalyst surface under high temperature environment, and is capable of removing amorphous carbon or other deposited carbon materials. However, the strength of this ability is closely related to the concentration, when the hydrogen content is too low, the etchability is insufficient, the amorphous carbon content is not

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reduced obviously, and the purity of the CNT is reduced, when the hydrogen content is too high, it may over-etch the catalyst and the CNT, resulting in a reduction of the product. Therefore, reasonable adjustment of hydrogen concentration can improve the purity of CNT while maintaining an appropriate growth rate[7].

Adjustment of the reaction gas flow rate is also critical to the growth rate and uniformity of CNT, Increasing the gas flow rate increases the concentration of carbon source gas and promotes the growth of CNTs, but too high a flow rate can lead to inhomogeneous growth. In addition, the system pressure also plays a regulatory role in the CNT growth process, with higher pressures inhibiting the growth of CNT diameter and lower pressures contributing to the increase in length. Optimization of these reaction conditions can significantly improve the yield and quality of CNTs.

In summary, the type of reaction gas, flow rate and system pressure have important effects on the growth efficiency and structural properties of carbon nanotubes, and optimization of these parameters is the key to improving the quality of CNT synthesis.

2.3. Reaction temperature and time

Reaction temperature and time are another crucial factor in the preparation of carbon nanotubes. They have important effects on the growth rate, structure, length diameter and overall quality of carbon nanotubes. Under high temperature conditions the decomposition rate of carbon source gas is accelerated, which provides more carbon atoms for the growth of carbon nanotubes and significantly increases the growth rate and yield of carbon nanotubes[8]. At the same time, the high temperature also promotes the optimization of the crystal structure, which leads to the improvement of the crystallinity and integrity of carbon nanotubes, reduces the degree of defects, and ultimately makes them exhibit good mechanical strength and electrical properties.

Conversely, the low decomposition rate of the carbon source gas at low temperatures reduces the growth rate, which in turn prolongs the preparation time and reduces the yield. Meanwhile, at low temperatures, the growth process of carbon nanotubes is difficult to control, and structural defects are more likely to appear, affecting the electrical conductivity and mechanical properties. Therefore, controlling the temperature within the reaction zone can regulate the length and diameter distribution of carbon nanotubes. That is, the high-temperature region is used to promote growth while the low-temperature region restricts growth, thus obtaining carbon nanotubes of specific lengths and diameters[9]. However, a uniform temperature distribution is crucial for the preparation of long-scale carbon nanotubes, and temperature fluctuations can lead to inconsistent growth rates, which affects the uniformity of length and diameter, and hence the quality of carbon nanotubes.

Extending the reaction time helps to increase the yield of carbon nanotubes, but also increases the risk of overgrowth, leading to a decrease in structural integrity and phenomena such as bending and bifurcation, which affects their performance. The growth rate of carbon nanotubes gradually decreases with the extension of reaction time, which is attributed to the decrease of active sites on the catalyst surface as the reaction proceeds. Thus, proper control of reaction time and temperature is an important way to optimise the carbon nanotube growth process[10]. In conclusion, the reaction temperature and time play a key role in the synthesis of carbon nanotubes and the rational adjustment of these parameters is crucial for increasing the yield and improving the structural properties.

3. Conclusions

The preparation process of carbon nanotubes (CNTs) is multiply affected by catalyst, reaction gas and reaction conditions. The selection and alloying of the catalyst significantly affect the growth rate and structural properties of CNTs, while the type and flow rate of the gas source and the concentration of the reaction gas play a crucial role in the quality of CNTs. In addition, the regulation of reaction

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temperature and time not only relates to the decomposition efficiency of the carbon source gas, but also directly affects the diameter and length distribution of CNTs. Therefore, optimization of these key factors can effectively improve the overall performance and synthesis efficiency of carbon nanotubes, which is of great practical significance to promote the application of CNTs in the field of high-performance materials and energy storage.

Authors Contribution

All the authors contributed equally and their names were listed in alphabetical order.

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