Journal of Electronic Research and Application, 2026, Volume 10, Issue 6
http://ojs.bbwpublisher.com/index.php/JERA
Online ISSN: 2208-3510
Print ISSN: 2208-3502

Research on the Controllable Growth Mechanism and Structural Characterization Methods of Single-Walled Carbon Nanotubes

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Abstract: As a typical one-dimensional carbon nanomaterial, single-walled carbon nanotubes (SWCNTs) possess a unique electronic structure, excellent mechanical properties, and outstanding thermal and electrical conductivity, showing important application value in cutting-edge fields such as nanoelectronic devices and composite materials. Structure determines properties, which is the core foundation for the application of SWCNTs. Their physicochemical properties are significantly affected by microstructural parameters such as diameter and chirality. Therefore, in-depth analysis of the controllable growth mechanism and research on precise structural characterization methods are of great significance for promoting the large-scale application of SWCNTs.

Keywords: Single-walled carbon nanotubes; Controllable growth mechanism; Structural characterization methods; Research progress

Online publication: Jul 23, 2026

1. Research the value of controllable growth and structural characterization of SWCNTs

1.1. Improving the growth theory system of low-dimensional carbon materials

SWCNTs are one-dimensional tubular nanostructures formed by rolling up graphene sheets. Their growth involves a series of reactions, including carbon source cracking, tube wall extension, and growth termination, which together constitute a typical vapor-liquid-solid (VLS) or vapor-solid-solid (VSS) interfacial catalytic reaction system [1]. Traditional theories of carbon material growth cannot fully explain the microscopic mechanisms at the nanoscale. Research on the controllable growth mechanism effectively fills the gaps in the basic theory of low-dimensional carbon materials. It improves the theoretical framework of nanocatalysis and low-dimensional material growth.

1.2. Unlocking the industrial application potential of SWCNTs

The physicochemical properties of SWCNTs are highly structure-dependent. Metallic SWCNTs exhibit excellent electrical conductivity suitable for high-performance conductive materials, while semiconducting SWCNTs possess superior on/off ratios and carrier mobility. Controllable growth technology enables precise regulation of diameter, chirality, and other parameters, producing high-purity samples with uniform structures that accurately match the requirements of different scenarios [2]. For example, single-chirality semiconducting SWCNTs can be used to construct ultra-high-speed, low-power transistors in the chip field; high-crystallinity SWCNTs greatly enhance the rate performance and cycle life of lithium batteries and supercapacitors in the energy field. Moreover, precise structural characterization methods significantly improve industrial quality control, enabling rapid detection of structural parameters and ensuring stability in large-scale production.

1.3. Promoting independent innovation of high-end nanomaterials

Low-dimensional carbon materials are a strategic focus of global competition in the new material sector. As a core representative material, the controllable preparation and precise characterization technologies of SWCNTs reflect a country's core competitiveness in nanoscience and technology. Currently, developed countries such as the United States, Japan, and South Korea hold leading positions in the controllable growth of chiral SWCNTs and the high-precision characterization of SWCNTs, gradually monopolizing core technologies and equipment [3]. Research on the controllable growth mechanism and structural characterization methods for SWCNTs helps overcome the bottleneck in precise structural regulation, establish a characterization technology system with independent intellectual property rights, and enhance China's international competitiveness in carbon nanomaterials. Furthermore, the development of SWCNT-controllable technologies drives the coordinated upgrading of upstream and downstream high-end industries, such as electronic information and new energy, thereby supporting the advancement of China's high-end manufacturing.

2. Research the status of the controllable growth mechanism and structural characterization of SWCNTs

2.1. Research status of controllable growth mechanism

2.1.1. Development and limitations of classical growth models

At present, chemical vapor deposition (CVD) is the most common method for preparing SWCNTs, and the classical VLS and VSS models primarily explain its growth mechanism. The early VLS model proposed that transition-metal catalysts (Fe, Co, Ni, etc.) melt into liquid droplets at high temperatures; carbon-source gases crack on the catalyst surface to form active carbon atoms, which dissolve and diffuse into the droplets. Upon saturation, carbon atoms precipitate and assemble into SWCNTs. This model provides a preliminary explanation of the growth process but fails to adequately account for chiral selectivity and precise diameter regulation [4]. The VSS model applies to high-melting-point solid catalysts such as W, Mo alloys, and metal carbides. Active carbon atoms adsorb, migrate, and nucleate on the solid catalyst surface, and lattice symmetry matching between catalyst crystal planes and SWCNT walls enables directional structural regulation. In recent years, the screw dislocation theory has improved our understanding of growth kinetics, stating that the SWCNT growth rate correlates positively with the number of active sites at the open end. However, follow-up studies found that this theory applies only to high-etchant-concentration systems, with

limited universality.

2.1.2. Research progress of structure-controllable growth

For diameter control, the academic community has reached a consensus: catalyst particle size is the core factor determining SWCNT diameter. By regulating catalyst particle size, linear controllable adjustment of diameter in the range of 0.8–3 nm can be effectively achieved. For chiral control, no complete breakthroughs have yet been achieved [5]. International research teams have improved chiral selectivity through substrate induction and electric field regulation, but 100% chiral purity remains unattainable.

2.1.3. Core existing problems

Currently, challenges in the controllable growth mechanism of SWCNTs in China include: an unclear atomic-scale interaction mechanism at the catalyst-SWCNT interface; unquantified thermodynamic and kinetic thresholds for chiral-selective nucleation; and complex coupling effects among temperature, atmosphere, catalyst state, and other parameters during growth, with no unified theoretical model [6].

2.2. Research status of structural characterization methods

SWCNT structural characterization mainly focuses on core parameters such as diameter, chirality, and length. Existing technologies fall into three categories: microscopic imaging, spectral analysis, and electron diffraction. The principles, application scenarios, advantages, and limitations of each technique are summarized in **Table 1**.

Table 1. Comparison of mainstream structural characterization methods for SWCNTs

Characterization method	Core principle	Measurable structural parameters	Core advantages	Main limitations
High-Resolution Transmission Electron Microscopy (HRTEM)	Electron beam penetrates the sample; atomic scattering forms lattice diffraction images	Diameter, tube wall defects, atomic arrangement	Atomic-level resolution, direct observation of microstructure	Complex sample preparation, electron beam damage, not suitable for batch testing
Scanning Tunneling Microscopy (STM)	Detects surface atomic morphology based on the quantum tunneling effect	Chirality index, atomic arrangement, and diameter	Ultra-high chiral accuracy, strong surface structure resolution	Only applicable to conductive samples, slow testing, and a small characterization range
Raman Spectroscopy	Inelastic scattering between photons and carbon atoms; characteristic peaks correspond to structural information	Diameter (RBM peak), defect density (*I*D/*I*G), chirality	Fast, non-destructive, batch characterization, easy operation	Limited chiral accuracy, difficult to distinguish similar chiralities
UV-Vis-NIR Absorption Spectroscopy	An electronic transition absorbs specific wavelengths that correspond to the electronic structure.	Diameter, metallic/semiconducting ratio, purity	Non-destructive, fast, quantitative analysis of the conductivity type	Cannot directly measure chirality, highly sensitive to high-purity samples
Nanobeam Electron Diffraction (NBED)	Electron beam diffraction forms characteristic patterns; lattice structure analysis.	Chirality index, lattice symmetry	High chiral accuracy, reliable results	Expensive equipment, complex testing, single-tube characterization only

2.2.1. Application progress of mainstream characterization technologies

Microscopic imaging is the core method for atomic-level structural characterization. HRTEM clearly observes tube wall defects and diameter uniformity, and can be combined with NBED for precise chirality index measurement. STM directly analyzes chirality through atomic-scale imaging, serving as an important standard for chiral characterization, but its low efficiency limits its use to basic laboratory mechanistic research [7]. Spectral analysis is the preferred choice for industrial characterization. Raman spectroscopy quickly determines diameter distribution via the inverse relationship between radial breathing mode (RBM) peaks and diameter. It quantitatively evaluates defect density using the *I*D/*I*G ratio, making it the most widely used rapid characterization method. UV-Vis-NIR spectroscopy efficiently distinguishes metallic and semiconducting SWCNTs, enabling quantitative analysis of conductivity-type ratios for rapid batch-sample screening.

2.2.2. Existing problems in the characterization field

Current structural characterization technologies face a trade-off between precision and efficiency. High-precision methods (STM, NBED) are slow and costly, failing to meet the needs of online detection in large-scale production. Meanwhile, rapid methods (Raman and absorption spectroscopy) lack precision, making it difficult to measure chirality accurately and to trace defects [8]. Additionally, China lacks unified characterization standards, leading to large deviations in test results across laboratories and equipment, with poor data comparability and interoperability.

3. Realization paths for controllable growth and structural characterization of SWCNTs

This section analyzes the controllable growth mechanism from three perspectives: multi-scale theoretical simulation, targeted catalyst optimization, and process parameter regulation. See **Table 2**, which shows the correlation between growth and characterization.

Table 2. Corresponding characterization table

Core chapter	Core technical points	Core functions
Construction of a multi-scale theoretical simulation system	Combine DFT, MD, MLFF to build a multi-scale simulation system; quantify temperature, atmosphere, etc.	Analyze elementary reactions, establish theoretical models, and provide comprehensive theoretical guidance.
Targeted design and optimization of catalysts	Design intermetallic compounds and supported catalysts; regulate crystal planes and particle sizes	Improve chiral selectivity, inhibit catalyst agglomeration, and provide catalytic support.
Multi-parameter synergistic regulation of growth processes	Optimize CVD processes; regulate carbon source/etchant concentrations; develop in-situ real-time technologies.	Reduce defects, improve sample uniformity, and realize closed-loop regulation.

3.1. In-depth analysis paths for controllable growth mechanism

3.1.1. Construction of a multi-scale theoretical simulation system

To achieve controllable growth of SWCNTs, a multi-scale growth simulation system ranging from the atomic to the macroscale can be established by combining density functional theory (DFT) and molecular dynamics (MD). DFT calculations can precisely analyze elementary reaction mechanisms, such as carbon-

source cracking and carbon-atom migration. MD simulations reveal atomic-scale interactions at the catalyst-SWCNT interface, uncovering crystal-plane matching and chiral-selective growth rules [9]. Furthermore, introducing machine-learning force fields (MLFFs) improves simulation efficiency, enabling large-scale, long-time growth-process simulations. This quantifies the effects of temperature, atmosphere, and other parameters on growth behavior, establishing a precise thermodynamic-kinetic coupled theoretical model to guide controllable growth.

3.1.2. Targeted design and optimization of catalysts

Break through the limitations of traditional transition metal catalysts and develop novel catalysts with precise structures. For example, prepare monodisperse intermetallic compounds with uniform size and regulate catalyst crystal planes and particle sizes to match the lattice symmetry of the target SWCNTs, thereby greatly improving chiral selectivity [10]. Meanwhile, develop functional supported catalysts, systematically optimize carrier-catalyst interactions, suppress high-temperature agglomeration, and establish more stable active growth sites.

3.1.3. Multi-parameter synergistic regulation of growth processes

Based on the carbon concentration regulation kinetic model and screw dislocation theory, systematically optimize CVD growth processes. Precisely control carbon source supply rate and etchant concentration: achieve chiral-selective growth using active site differences in high-etchant systems, and terminate non-target structure growth by regulating carbon source concentration in low-etchant systems [11]. Optimize reaction temperature and heating rate to balance nucleation thermodynamics and growth kinetics, effectively reducing defect formation. Additionally, develop in situ, real-time growth technologies for dynamic monitoring and closed-loop regulation of growth parameters, thereby significantly improving the structural uniformity of samples.

3.2. Construction paths for precise structural characterization methods

3.2.1. Integration of high-precision and high-efficiency characterization technologies

Establish a two-stage characterization system of “rapid screening + precise calibration”. The first stage uses rapid methods such as Raman and UV-Vis-NIR spectroscopy for preliminary screening of diameter, defect density, and other parameters, quickly eliminating unqualified samples. The second stage employs high-precision techniques (HRTEM-NBED, STM) to accurately measure chirality and atomic structure of high-quality samples, balancing efficiency and precision [12]. Meanwhile, develop multi-technology-combined characterization platforms that integrate spectroscopy, imaging, and diffraction to enable simultaneous multi-parameter characterization on a single device, thereby simplifying testing processes and improving data reliability.

3.2.2. Intelligent characterization and establishment of standard systems

Introduce machine learning to assist in the in-depth analysis of characterization data. Train deep learning models to automatically identify characteristic peaks in Raman and absorption spectra, rapidly inverting diameter, chirality, and other parameters [13]. Machine learning algorithms process electron microscopy images to automatically extract key information such as atomic arrangement and chirality index, reducing human error and improving data processing efficiency.

3.2.3. Development of in-situ and online characterization technologies

Targeting research on growth mechanisms and industrial quality control, with a focus on developing in situ and real-time characterization technologies. Use in-situ TEM and in-situ Raman spectroscopy to observe atomic migration, nucleation, and extension during SWCNT growth, verifying mechanisms and revising theoretical models [14]. Meanwhile, design online characterization modules integrated into CVD equipment to enable real-time monitoring and feedback-based regulation of structural parameters during growth, ensuring structural stability in large-scale production.

3.3. Collaborative development paths of mechanism research and characterization technology

Controllable growth mechanism and structural characterization research are mutually supportive. Precise characterization obtains structural evolution data during growth, which is used to invert mechanisms, revise theoretical models, and provide experimental evidence for growth parameter optimization [15]. Furthermore, build an industry-university-research collaborative innovation platform that integrates the theoretical advantages of universities and research institutes with the industrial experience of enterprises, effectively transforming laboratory-precise, controllable growth technologies into industrial mass production.

Disclosure statement

The authors declare no conflict of interest.

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