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Mechanisms, simulation methods, and application analysis of carrier transport properties in doped semiconductors

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Abstract. The semiconductor industry has evolved through multiple generations, with doping serving as a core approach to modulate semiconductor performance. It directly determines the key performance of electronic and energy devices, and its regulatory mechanisms, simulation methods, and applications have long been research focuses of academia. Clarifying the carrier transport mechanisms in doped semiconductors is crucial for promoting the continuous advancement of devices. This study focuses on the mechanisms and applications of carrier transport in such materials, employing literature analysis, case study, and comparative analysis methods. It systematically summarizes three core regulatory rules for semiconductors: the modulation of scattering mechanisms in traditional wide-bandgap inorganic semiconductors, quantum confinement and interface characteristics of ultra-wide-bandgap two-dimensional semiconductors, and density of states optimization in organic semiconductors. Additionally, this paper sorts out the applicable scenarios and multi-field applications of the relevant technologies, refines the cross-system carrier transport theory, and provides a comprehensive and practical reference for the design of various semiconductor devices.

Keywords: semiconductor, doping, transportation, simulation, carrier

1. Introduction

The semiconductor industry has evolved through generations, from silicon-based and wide-bandgap semiconductors to organic semiconductors. As a core approach to regulating carrier transport properties and break bottlenecks in device efficiency and reliability, doping, along with its regulatory mechanisms, simulation methods and practical applications, has long been an academic focus. Previous studies have achieved progress: Li [1] analyzed scattering mechanisms (alloy disorder, ionized impurities) in AlInGaN heterojunctions, clarifying Al/In composition matching rules to optimize mobility; Xin et al. [2] summarized preparation processes of ultra-wide-bandgap 2D semiconductors, revealing the synergistic effect of quantum confinement and Van der Waals interfaces on carrier transport and defect doping strategies; Qin [3] proposed a positively skewed Density of States (DOS) model, breaking the limitations of traditional Gaussian/exponential DOS to accurately fit transport properties of organic semiconductors across all concentrations. However, existing research mostly focuses on individual systems, lacking systematic integration of cross-system transport mechanisms, simulation methods and application scenarios. This makes it difficult to form a full-dimensional

regulatory framework. Thus, this study, via literature review, case comparison and cross-system induction, analyzes transport mechanisms, sorts out mainstream simulation methods and discusses multi-field applications, establishing a complete logical chain of doping regulation, transport mechanism, simulation method, and device application. This study fills the gap of traditional reviews and provides comprehensive theoretical and practical guidance for cross-system semiconductor optimization and new device design.

2. Carrier transport mechanisms in doped semiconductors

2.1. Carrier transport mechanisms in inorganic semiconductors

2.1.1. Traditional wide-bandgap inorganic semiconductors

Li [1] found that material scattering mechanisms directly determine carrier mobility, concentration and transport stability, thereby affecting key device performance such as conductivity and breakdown voltage, and are the core factors limiting transport efficiency. As is depicted in Table 1 that in AlInGaN heterojunctions, alloy disorder scattering mobility, dominated by alloy scattering potential, is affected by 2DEG concentration and infiltration probability: scattering intensifies with increasing Al content, and optimizing Al/In ratios balances device performance. They also found that mobility peaks when Al and In compositions fluctuate independently with the same amplitude and direction, while scattering is strongest with opposite fluctuation directions. Table 1 illustrates that in H-terminated diamond, surface ionized impurity scattering causes low 2DHG mobility. Excessive scattering from double-gate dielectrics is reduced by optimizing dielectric parameters. Doping in both AlInGaN and H-terminated diamond weakens scattering by regulating carrier concentration and interface states, thus enhancing carrier transport efficiency.

2.1.2. Ultra-wide-bandgap two-dimensional inorganic semiconductors

Xin et al. [2] showed that carrier transport properties of ultra-wide-bandgap 2D inorganic semiconductors are jointly dominated by quantum confinement effects and van der Waals interface characteristics. It can be observed from Table 1 that quantum confinement induces significant anisotropy in mobility, while the dangling-bond-free van der Waals interfaces reduce interface state scattering and defect trapping, lowering carrier transport losses. As demonstrated by the data in Table 1, the lattice and defect scattering still affect transport efficiency, with defect scattering being the main limiting factor at low carrier concentrations. Doping is a core means to enhance efficiency: N-doping converts intrinsic insulating or n-type Ga_2O_3 to p-type, addressing the p-type doping challenge of ultra-wide-bandgap materials and improving Ultraviolet (UV) detector responsivity. Defect doping (e.g., oxygen vacancies in ZnO) flexibly adjusts carrier concentration, balancing the trade-off between mobility and concentration. It also passivates native defects, reducing carrier trapping and scattering, strengthening the transport advantages of van der Waals interfaces, and ultimately achieving synergistic improvement in mobility and device performance.

2.2. Carrier transport mechanisms in organic semiconductors

Qin [3] showed that carrier transport in organic semiconductors is dominated by hopping transport, with the local-extended state distribution of Density of States (DOS) as the core regulatory factor. As is shown in Table 1 that traditional Gaussian DOS leads to 1-2 orders of magnitude deviation in mobility calculation at high carrier concentrations, while exponential DOS fails to fit the stable mobility at low concentrations. Their proposed positively skewed DOS model achieves accurate fitting across all concentrations by optimizing the local-extended state ratio, essentially solving the DOS-carrier transport mode matching issue and providing key support for the directional regulation of organic semiconductor transport efficiency.

2.3. Cross-system mechanism comparison

Core differences in cross-system carrier transport mechanisms lie in dominant regulatory mechanisms and optimization goals. As is shown in Table 1 that traditional wide-bandgap inorganic semiconductors focus on heterojunction scattering suppression, weakening scattering by optimizing alloy composition and lattice matching, with doping requiring a balance between composition and scattering intensity. From Table 1, we can see that ultra-wide-bandgap 2D semiconductors leverage quantum confinement and van der Waals interface advantages. Doping needs to balance quantum confinement and interface coupling while passivating defects to enhance transport. As is shown in Table 1 that organic semiconductors, dominated by hopping transport, rely on regulating the local-extended state ratio of DOS, with doping balancing carrier gain and disorder. All three regulate carrier concentration via doping, but their core balance goals differ due to material structural variations.

Table 1. Comparison table of three semiconductor carrier transport mechanisms

Comparison Dimension	Traditional Wide-Bandgap Inorganic Semiconductors	Ultra-Wide-Bandgap 2D Inorganic Semiconductors	Organic Semiconductors
Regulation Mechanism	Heterojunction scattering suppression	Quantum confinement and van der Waals interface characteristics	Hopping transport and density of states distribution regulation
Limiting Factors	Alloy disorder/ionized impurity scattering	Defect scattering/lattice scattering	Hopping transport loss in disordered systems
Doping Effect	Weakens scattering and improves transport efficiency	Adjusts concentration, passivates defects, and strengthens interfaces	Optimizes density of states ratio to adapt to full-concentration transport
Key Parameters	Al/In composition, dielectric layer parameters	Interlayer coupling strength, defect concentration	Density of states distribution shape, molecular packing density

3. Simulation methods for carrier transport in doped semiconductors

3.1. Simulation methods for inorganic semiconductors

3.1.1. Simulation methods for traditional wide-bandgap inorganic semiconductors

When studying carrier transport in traditional wide-bandgap inorganic semiconductors, Li [1] adopted a multi-scattering mechanism coupling model. As depicted in Figure 1 that for AlInGaN/AlGaN heterojunctions, they integrated core mechanisms like alloy disorder and composition fluctuation scattering, analyzing five fluctuation scenarios and finding optimal mobility when Al and In compositions fluctuate independently with the same amplitude and direction For H-terminated diamond, they focused on the dominant role of surface ionized impurity scattering in 2DHG transport. For double-gate dielectric structures, Remote Interface Roughness (RIRS) and Remote Coulomb Scattering (RCS) were additionally coupled. Under high-field conditions, Hot Phonon Effect (HPE) and conduction band non-parabolicity were incorporated to quantitatively analyze their modulation of carrier energy and momentum relaxation times in GaN, AlN and InN, providing key theoretical support for optimizing high-voltage, high-frequency devices. As is shown in Figure 1 that doping process simulation and optimization are achievable via SRIM software [4], which employs the Monte Carlo method to accurately simulate ion implantation range, distribution and damage.

Combined with mathematical models, it calculates sputtering loss and buried layer thickness, with simulation-experiment deviation within 10%.

3.1.2. Simulation methods for ultra-wide-bandgap two-dimensional inorganic semiconductors

Xin et al. [2] adopted a coupled simulation method of "quantum confinement combined with interface optimization" for ultra-wide-bandgap inorganic semiconductor carrier transport. As is illustrated in Figure 1 that for van der Waals layered materials, they solved the Schrödinger-Poisson equations self-consistently to quantify quantum confinement and optimize interlayer coupling-defect scattering competition. For non-layered materials, they coupled defect scattering and high-field hot phonon effects, establishing a process-transport performance mapping model to support device optimization.

3.2. Simulation methods for organic semiconductors

Qin [3] adopted a "Density of States (DOS) optimization combined with analytical master equation" method to study carrier transport in organic semiconductors. As is shown in Figure 1 that they proposed unified and novel positively skewed DOS models, breaking the limitations of traditional Gaussian and exponential DOS to accurately fit mobility across the full carrier concentration range and wide electric field scope. Based on the Miller-Abrahams hopping theory, they constructed mobility models for zero-field, high-field and doping scenarios, and established two semi-analytical Seebeck coefficient models suitable for high-concentration and doped conditions. This work provides key theoretical support for the performance optimization and molecular design of organic field-effect transistors and thermoelectric devices.

3.3. Cross-system comparison and adaptation scenarios of simulation methods

Cross-system carrier transport simulations for semiconductors adhere to the core logic of mechanism, modeling-parameter, quantification-experimental, and validation with scenario-specific adaptations. Figure 1 displays that traditional wide-bandgap inorganic semiconductors adopt multi-scattering coupling models, integrating alloy disorder and polar optical phonon scattering, and considering interface roughness and high-field hot phonon effects, suitable for complex scattering in high-voltage High Electron Mobility Transistors (HEMTs) and power switches. Ultra-wide-bandgap 2D inorganic semiconductors focus on quantum confinement and defect scattering fitting, adapting to low-dimensional transport in UV detectors and flexible devices. Organic semiconductors prioritize DOS optimization and analytical master equations, using positively skewed DOS models to fit hopping transport across all concentrations and electric fields, supporting organic Field-Effect Transistors (FETs) and thermoelectric device design. All simulations are validated employing the four-probe method [5]. Semi-infinite and infinite thin-layer models are applied for bulk inorganic and 2D/organic semiconductors, enabling accurate doping concentration measurement as a key link between simulation and experiment.

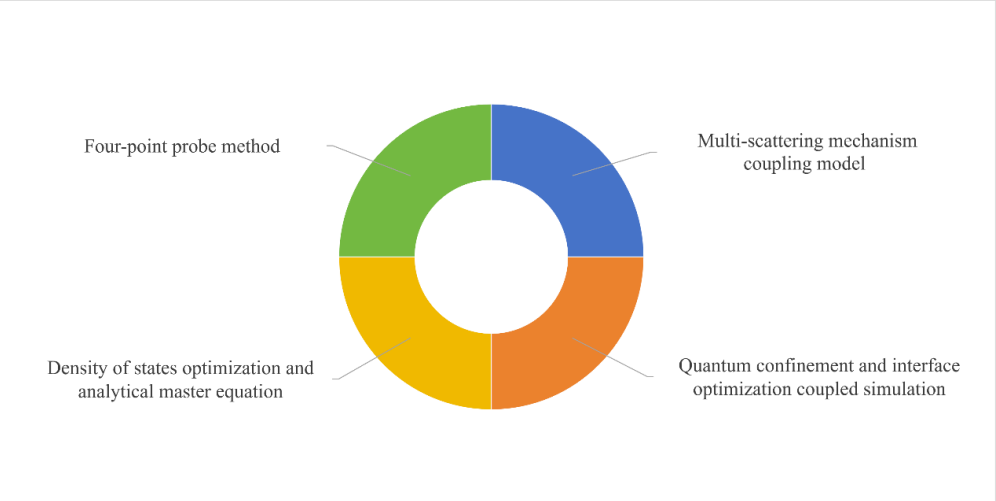

Figure 1. Simulation methods for carrier transport in doped semiconductors

4. Application analysis of carrier transport in doped semiconductors

Doped semiconductors have achieved critical performance breakthroughs in high-voltage electronics, ultraviolet detection, flexible electronics, and other fields through the precise regulation of carrier transport properties.

4.1. Applications of traditional wide-bandgap inorganic semiconductors

Traditional wide-bandgap inorganic semiconductors occupy a core position in high-voltage devices due to their low scattering characteristics and high breakdown voltage. AlInGaN heterojunctions stand out particularly: optimizing the Al/In composition ratio effectively suppresses alloy disorder scattering, thereby improving carrier mobility and device voltage withstand capability. Chen [6] replaced the barrier layer with a new quaternary alloy, optimized its composition and reduced its thickness, which suppressed alloy disorder scattering, mitigated the short-channel effect, and significantly enhanced the performance of AlInGaN heterojunction power modules. These modules achieve a breakdown voltage exceeding 1.2 kV and a 60% reduction in switching loss, and are now widely applied in key fields such as new energy vehicle inverters and smart grid converter stations. For H-terminated diamond, precise doping controls the 2DHG concentration, effectively weakening surface ionized impurity scattering and achieving a high carrier mobility of up to 2000 $cm^2 \cdot V^{-1} \cdot s^{-1}$ [7]. This excellent property allows H-terminated diamond devices to operate stably at extreme temperatures above 300 °C [7], fully meeting the stringent requirements of aerospace, petroleum exploration and other fields for high-temperature, high-reliability power electronic devices.

4.2. Applications of ultra-wide-bandgap two-dimensional inorganic semiconductors

Ultra-wide-bandgap two-dimensional inorganic semiconductors exhibit prominent advantages in Ultraviolet (UV) detection and flexible electronics, thanks to their quantum confinement effects and low transport loss at van der Waals interfaces. A Metal-Semiconductor-Metal (MSM) deep-UV photodetector based on Gallium Oxynitride (GaON), fabricated via a Plasma-Enhanced Chemical Vapor Deposition (PECVD) system, demonstrates high responsivity (0.327 A/W), ultrahigh detectivity (4.08×10^{14} Jones), and fast response speed (rise/fall times of 0.708 s/0.413 s). This makes it excellent for high-voltage arc detection and industrial safety applications [8]. ZnO-based flexible materials show unique potential in UV detection and piezoelectric

sensing. Zhang et al. [9] prepared a ZnO@PAN flexible composite nanofiber membrane via electrospinning, utilizing the synergistic piezoelectric effect between ZnO nanorods and PAN fibers to develop a self-powered flexible pressure sensor with high output performance. The device maintains stability under bending deformation, delivering an open-circuit voltage of 5.5 V and a short-circuit current of 0.61 μA. Its performance remains unchanged after 5000 cyclic tapping tests, enabling applications in wearable devices, flexible sensing terminals, and other emerging industries.

4.3. Applications of organic semiconductors

Carrier transport in organic semiconductors is dominated by the hopping mechanism, and their performance optimization can achieve full-concentration-range carrier regulation via positively skewed DOS models [3]. Wang et al. [10] optimized molecular packing density through backbone and side-chain engineering, and combined dynamic hydrogen bond networks with nanoconfinement effects. This enabled intrinsic stretchable organic semiconductors to exhibit low-cost and high-flexibility advantages in Organic Field-Effect Transistors (OFETs) and thermoelectric devices. For instance, pentacene derivative devices achieved an on/off ratio exceeding 10^6, while solution processing reduced costs by more than 50%. Meanwhile, the unique π-conjugated structure endows organic semiconductors with great potential in flexible electronics and spintronics, but their performance breakthroughs highly rely on the precise regulation of molecular orientation and microstructure. Zhou [11] utilized a strong magnetic field-assisted Solvent Vapor Annealing (SVA-HMF) technique to achieve highly oriented molecular chains in P (NDI2OD-T2) films, improving the Organic Field-Effect Transistor (OFET) mobility to 0.68 $cm^2 \cdot V^{-1} \cdot s^{-1}$ with an anisotropy of 59. This technique also enhanced the stability of PDI radical ferromagnets, providing high-performance material solutions for applications such as flexible displays and near-infrared detection.

5. Conclusion

This paper reviews the mechanisms, simulation methods, and practical applications of carrier transport in doped semiconductors, revealing the core laws of cross-system regulation: traditional wide-bandgap inorganic semiconductors suppress scattering by optimizing alloy compositions, ultra-wide-bandgap two-dimensional semiconductors reduce transport loss through quantum confinement effects and van der Waals interfaces, and organic semiconductors achieve full-concentration-range transport regulation relying on positively skewed Density of States (DOS) models. Cross-system simulation methods integrate multi-scattering mechanism coupling, quantum confinement-interface optimization, and analytical DOS master equations, thereby providing theoretical support for the design of devices including high-voltage High-Electron-Mobility Transistors (HEMTs) and flexible ultraviolet detectors.

However, this study has several limitations. Firstly, the literature selection is not comprehensive enough: only organic and inorganic classifications were adopted for literature retrieval and comparative analysis, without in-depth research on subcategories within different material systems (e.g., narrow-bandgap organic semiconductors), leading to incomplete coverage of certain special doping types. Secondly, cross-system comparisons are confined to macroscopic parameters, lacking in-depth analysis of detailed parameters, which may cause deviations in predicting carrier transport behavior in actual devices. Additionally, existing research mostly focuses on transport characteristics under static conditions, with few studies on the response mechanisms of doped semiconductors in dynamic environments (e.g., temperature gradients and electric field transients). This limits their application potential in scenarios such as high-frequency power electronics.

In the future, research can be advanced in the following aspects: expanding studies on subdivided material systems, deepening parameter analysis, exploring transport response mechanisms under dynamic environments, improving cross-system theories and simulation methods, and advancing application breakthroughs of doped semiconductors in high-frequency power electronics and other fields.

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