

Quantum Semiconductor Devices: Current Progress and Future Trends

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Abstract

Modern electronics are frequently used in quantum semiconductor devices. The devices are extremely small and their behavior cannot be described by traditional theories. The impacts include quantum confinement and tunneling. Several new quantum devices have been proposed in the past, including an examination of their theory and design. Additionally, new modeling methods are being developed. Atomic-scale production has been shown to be constantly increasing. This effort addresses several issues at the same time. As a result, the device's dependability remains a challenge, produce variations have an impact on performance, cooling and thermal management are not easy to perform. This study reviews recent achievements in quantum semiconductor devices. It discusses device characteristics, modeling and production methods. It also identifies current disadvantages and unsolved challenges that minimize future effort are addressed in detail.

Keywords: Quantum Semiconductor Devices, Quantum Confinement, Device Modeling, Atomic-scale Production, Quantum Transport, Future Trends.

1. Introduction

Modern electronic systems are based on semiconductor devices which are used in computers. Their applications are found in communication systems, medical devices and energy systems. Scaling will improve the performance of devices which reduce transistor sizes and power consumption. The switching speed was also increased and it is used in large devices [1]. The development with traditional semiconductor theory discusses the movement of carriers, drift and diffusion.

Device performance transitions from classical to quantum are determined by rapid reduction in feature size at successive technological nodes within semiconductor technology. Now-a-days, integrated circuits are manufactured at the deep submicron/nanometer range with node examples of 90nm, 65nm, 45nm, 32nm, 22nm, 14nm, 10nm, 7nm. As feature sizes have progressed to below 20nm, short-channel effects, gate leakage, variability and quantum effects had an increased impact due to reduction in size. Quantum confinement, direct transfer from source to drained tunneling, and distinct energy states become a key problem in the field of carrier transport. The changes associated with these physical limitations at their associated nodes have led to innovation in devices will be architected and also created innovative concepts for quantum semiconductors and improved modeling capabilities.

The size of devices reduced to nanometers in recent years. The electrons fail to act separately as particles. The importance of tunnelling increases make significant behaviour of waves and the level of energy become discrete. These effects modify the reliability and functioning of the devices. This change affects the production of quantum semiconductor devices. which are based on quantum mechanical principles [2]. Their actions lack to explain traditional theory. The history of the development of quantum concepts is illustrated in figure 1.

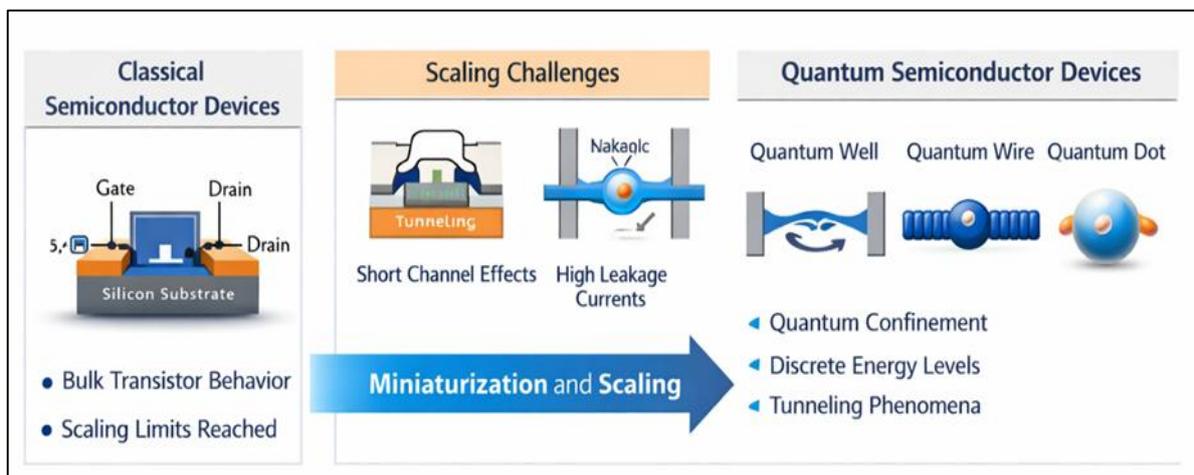


Figure 1. Evolution of Quantum Technologies

The above timeline shown in figure 1 provides a high-level overview of stages in the development of quantum technologies using semiconductors. It begins with the principles of quantum mechanics, such as wave-particle duality and quantization applied to the movement of an electric charge at an atomic level. The next level was the development of band theory and

quantum tunneling provided the foundation for nanoscale devices. The another stage was the production of low-dimensional semiconductor structures (quantum wells, wires, and dots), provided definitive evidence for the existence of confinement effects. The final stage on the timeline shows the development of atomic-scale structures, individual electron manipulation and realization of qubits with semiconductors over time. These timelines depict a gradual progression from the theoretical realm of quantum-physics to the practical domain of quantum-device engineering in semiconductors.

Quantum semiconductor devices have multisectoral application areas. It utilized for computing, sensor applications, communication application and energy conversion application. Each of these application areas are rapidly advanced and new device concepts are emerging every year. The fabrication process and the modeling tools are more accurate. However, there are few challenges with these devices. Scalability, temperature management and variability are the two major problems. A systematic investigation of the current trends and advances in the field is required to handle the current challenges in the industry.

Quantum semiconductor devices are used in applications where quantum processes are controlling due to the visibility at minor device sizes. An example of a quantum process is quantum confinement restricts how far a carrier can move and produces discrete energy levels. Another example of a quantum phenomenon is tunneling allows a carrier to tunnel using the challenge. The tunneling phenomenon is not predicted using classical theory.

Several classifications define devices that are classified as quantum semiconductor devices, including quantum dots are characterized by having carriers surrounded them at all angles. The confinement of carriers occurs along one dimension in 'quantum wells.' Carrier quantities can be manipulated and controlled using single electron devices, as the individual charge is targeted through controlled penetration of barriers and by employing tunnel-based devices. Devices utilizing atoms are manufactured by accurately placing dopants. Each device has its unique features and devices include their own benefits [3].

These devices have low power consumption. They are highly sensitive, enabling quantum data processing. At the same time, they introduce new constraints on the devices as their performance is dependent on defects in the device. The device performance will impact on minor variations. External noise may affect the stability of devices. All of these issues must be examined and controlled during the development of quantum semiconductor devices. [4].

Quantum semiconductor devices are applicable to a wide range of applications, including computing, sensing, communications and energy conversion. This sector has expanded rapidly with new device designs introduced every year. Production technologies have improved accuracy over the years. The tools for modeling device performance are becoming significantly more accurate. Considering this rapid advancement, there are still challenges involved with quantum semiconductor devices. Scalability remains an issue, with varying yields, and temperature control is also a significant challenge. There is a need for an extensive assessment of current advances and future directions of research and development for quantum semiconductor devices.

1.1 Overview of Quantum Semiconductor Devices

The control of quantum mechanics results in quantum mechanical devices. Quantum confinement of charge carriers is found in small dimension devices, resulting in unique electron behavior. Tunnelling is another example of how charge carriers operate according to quantum theory.

The various types of devices that use quantum mechanics to produce their operation are referred to as quantum semiconductor devices. A quantum dot is a device that confines charge carriers in three-dimensional space; a single electron device controls the charge of a single electron and a quantum well confines charge carriers to a single direction. Many atom-based quantum devices depend on the precise arrangement of the dopants used to produce their operation, while tunnelling quantum devices take advantage of a controlled barrier penetration to allow charge carriers to tunnel through the barrier. Each class of device has unique characteristics and provides specific benefits.

Quantum semiconductor technology has the ability to provide new functionalities. Quantum semiconductors enable quantum data processing capabilities, improved sensitivity and low power operation of various types of devices including sensors, transistors, and electronic devices. Quantum semiconductors also have their own set of constraints. Defects may influence how a given quantum semiconductor behaves even through relatively small variations in that device is designed or developed. Additionally, an external noise will influence a semiconductor's stability as a result, attention must be provided when developing a quantum semiconductor.

1.2 Fundamentals of Quantum Mechanics in Semiconductors

A theory of Quantum Level-Wave functions describes the behaviour of all carriers within semiconductor devices at low dimensions. At the electron level, electrons behave as "wave functions", which are not "particles". Their energy does not have a continuous range, but consists of distinct levels. The momentum of the electron can be measured but cannot be measured precisely in space and time. These quantum features can have a significant effect when carriers transit through devices and the overall distribution of charge across the semiconductor material, hence the total current flow commonly inconsistent with classical predictions.

Thermal effects contribute significantly to the stability of quantum semiconductor devices' operation. Temperature change affects both carrier energy distribution, phonon interaction and scattering processes that affect coherence, tunneling and leakage currents. By increasing temperature, the ability of carriers to excite and combine the phonons will also increase, thus resulting in increased expansion of the energy levels and lower efficiency of quantum confinement. As these effects increase the rate at which coherence is lost and affecting the reliability of appropriate operation for these devices, there is an increased need for thermal control over many quantum devices achieve stable quantized states and predictable transportation behavior; therefore, maintaining the thermal management will be an essential characteristic of the design of quantum semiconductor systems.

The Schrodinger equation plays an important role in analyzing quantum semiconductors and is used to determine the atomic and electronic properties of carriers in confined structures. It also provides a description of the energy and wave functions of carriers in confined structures. The Poisson Equation provides a description of the electrostatic potential in the device. The Poisson and Schrodinger equations are generally solved together (self-consistently) for the analysis of practical devices; this self-consistent modeling is crucial when predicting the performance of quantum semiconductor devices. At the quantum level, traditional classical transport laws are inadequate to explain what occurs in quantum semiconductors. There are some additional phenomena occur at the nanoscale that affect the performance of devices: for example, quantum tunneling can enable carriers to expand across possible challenges that prevent their movement under normal classical conditions. Some devices utilize this tunneling phenomenon to achieve enhanced functionality such as rapid switching and lower operating voltage. The tunneling results in undesired leakage currents.

These leakage currents decrease efficiency of devices and regional isolation. Tunneling effects become more challenging to manage as the devices' size decreases. The quantum behavior of semiconductor devices is also affected by thermo-effects. The carrier energy distribution varies with change of temperature. The stimulation and leakage of carriers increase as the temperature raises. It also found that many quantum devices require cooling to be stable. The combination of these physical effects that forms the fundamental operational limitations of quantum semiconductor devices. [2], [3].

1.3 Development of Classical to Quantum Devices

Over the years, electronic devices were operated using classical semi-conductor electronic devices. The electronic device industry was established using traditional bulk carrier transport technology. Device designers depend on scaling laws to determine performance and improve device density. The growth of the number of transistors on a chip was expected to exceed a specific rate and could be explained by Moore's Law until the rate began to decrease because of additional scaling. Scaling based on Moore's Law has decreased because the scale of the electronic component has approached the limits of fundamental physical limitations; For example, short-channel effects, leakage currents and the variability limits imposed by device size (e.g. the die dimension of $1\mu\text{m}$). As a consequence, the physical constraints on device functioning are predicted to be increasingly severe in areas of high technology. When devices become manufactured at deep nano scale, the operating principles of the devices will be affected by new physical phenomena. The challenges for manufacturing at the nanoscale become significant. There was an increase in short channel effects making them more challenging to control, there was an increase in leakage currents, making energy savings insufficient. Due to the increased variability and its effect on device behaviour, designers not able to manage to ignore quantifiable mechanical behaviour. This step indicated the beginning of the transition from classical semiconductor devices to quantum-dominant devices.

Quantum semiconductor devices not constitute an easy transition from classical devices; new device architectures that account for quantum confinement and tunnelling effects will be required. New materials may be required in order to create a stable quantum operation. The manufacturing process will have to possess atomic precision. In addition, a quantum mechanical treatment of charge carriers must be used for modelling purposes since classical design principles are insufficient. The transition is not yet complete and most devices currently

combine classical and quantum elements. This transition is an important for the development of future semiconductor technologies [6]. The interrelationships shown in Figure 2 highlight the connections between scaling of devices, development of quantum effects, complexity of modelling and the necessity for increased precision in production.

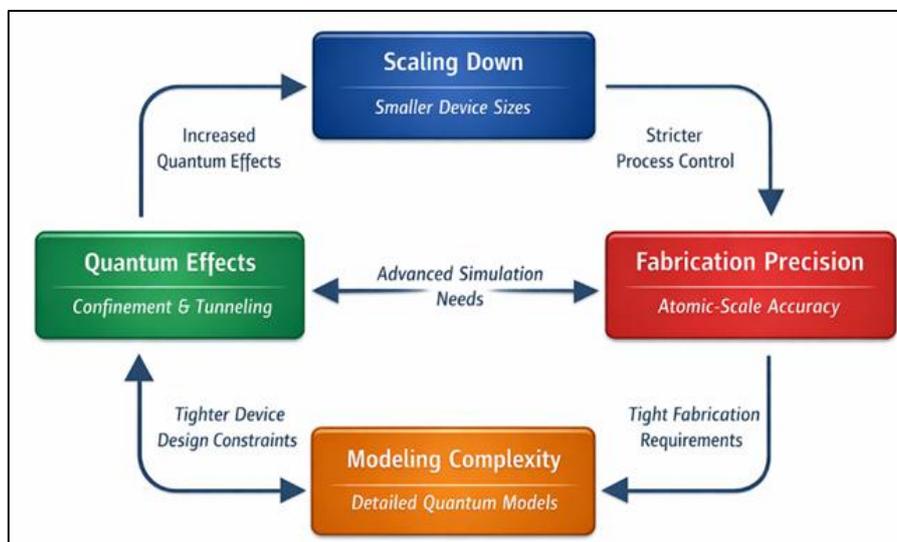


Figure 2. Relationship Between Device Scaling, Quantum Effects, Modeling Complexity and Accurate Production in Quantum Semiconductor Technologies

1.4 Motivation and Scope of the Survey

Quantum semiconductor devices have been the focus of extensive research in recent years with multiple articles published on a variety of topics. The majority of the research has focused on either the device's physical features or the methodologies used to study and simulate its behavior. Some of the evaluations focused with production and materials. Several research has included system-level integration into their analyses. As a result, the field is not completely unified and the majority of research have been evaluated independently each other. As a result, it is important to have a complete understanding of quantum semiconductor devices. This perspective should connect the fundamental particles of quantum semiconductors to the structure of real quantum semiconductor devices. Furthermore, this approach should connect the modelling techniques used for quantum semiconductor devices to the approaches utilized for producing quantum semiconductor devices. This viewpoint should also provide the key challenges to the continual growth of quantum semiconductor devices in a simple and systematic way. Finally, this should also present future directions for research that will

contribute to advancing the understanding of this area of research. The work has been provided is designed to fulfil these requirements.

The scope of this study includes a multitude of important areas associated with quantum semiconductor devices from the fundamental theory behind their quantum transport properties; modeling and simulation methods of analyzing devices; new device architectures; new production methods; reliability issues; thermal management issues and future trends, challenges and opportunities. The primary goal is to provide a single source of data that researchers and engineers in this field may easily access.

2. Fundamentals of Quantum Semiconductor Device Theory

Quantum mechanics describes the behavior of charge carriers in semiconductor devices is dominated by the principles of quantum theory. Classical drift-diffusion theory becomes invalid when dimensions decreased below one nanometer, e.g. at the atomic scale. Theoretical studies like [3] indicate that carrier transport (movement), energy distribution, and carrier/ electrostatic interactions are fundamentally quantum mechanical. As a result, many of the properties or functions of chronic quantum semiconductor devices are determined, or 'controlled', by three physical mechanisms (rather than by bulk transport): confinement of charge carriers, tunneling of charge carriers (in contrast to drift), and discrete energy-level states (in contrast to freeband energy). A detailed understanding of the basic concepts behind these devices is required to accurately model, produce, or integrate complex quantum semiconductor devices.

2.1 Quantum Confinement Effects in Semiconductor Structures

Quantum confinement results occurs when a certain dimension of a semiconductor structure is similar to the wavelength of the carriers. In these situations, the carriers' movements are spatially confined results in a huge modification of an electronic structure. The overall confinement of nanostructures explained in [14] provides proof for confinement leads to the development of discrete levels of energy as opposed to continuous bands of energy. The amount of confinement is based on the geometry, composition of the material and quality of the interface. Figure 3 provides a description of the idea of quantum confinement shows discrete energy levels and confined carrier motion in quantum wells, quantum wires, and quantum dots.

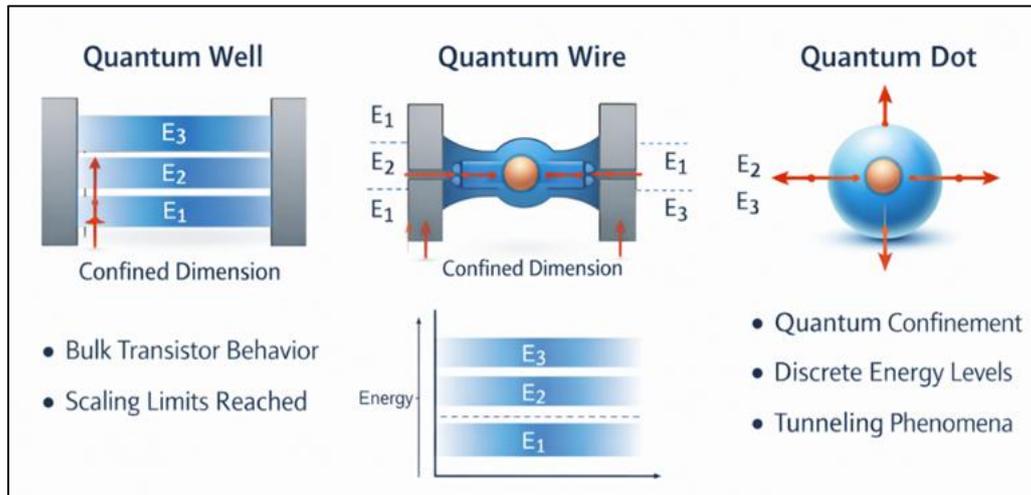


Figure 3. Quantum Confinement in Semiconductor Nanostructures

Quantum wells, quantum wires and quantum dots are confinement geometries that exist in modern nanostructure production. Quantum wells restrict movement in one dimension and allow the carriers to move freely over the plane. Quantum wires restrict movement in two dimensions. Therefore, they further restrict the carriers' ability to move around. Quantum dots restrict movement in all three dimensions, resulting in an atom-like electronic energy spectrum. The experimental and theoretical observations covered in [13] shows that quantum dots made from atoms have highly stable confined states when production methods are closely monitored.

Under the accurate set of boundary conditions, the Schrodinger equation can be solved analytically to give the effects of quantum confinement. Considering a particle enclosed in an optimum one-dimensional potential well whose width is L , the quantized energy levels are given as:

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2m^* L^2}, n = 1, 2, 3, \dots \quad (1)$$

where m^* is the carrier effective mass.

Extension to higher-dimensional confinement yields discrete subband structures, where the total energy becomes:

$$E_{n_x, n_y, n_z} = \frac{\hbar^2 \pi^2}{2m^*} \left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2} \right) \quad (2)$$

Interfacial energy quantization (i.e., quantitative measurement of kinetic energy related to electronic state) decreases proportionally in device size. This decrease in geometric

dimension leads to increases in carrier transport, transition energies between bound and free states and other operational characteristics. Subband separation increases, in a huge dimensional structure of a device is decreased.

Quantum confinement has a direct effect on both the electrical and optical properties of materials. The structure of the confined energy will determine different behaviors associated with the material such as carrier density, mobility and transition energies. For example, quantum dots have demonstrated improved absorption and carrier separation due to confinement effects when used within photovoltaic solar cells as shown by the graphs provided in [18]. Additionally, the devices have a decreased sensitivity to size variation and thus develop large shifts in energy levels as a result of small production defects, as demonstrated by the quantum confined nanostructures discussed [14].

The dimensionality of quantum confinement has a substantial influence on both the carrier and threshold behavior, as it has a direct impact on the density of states (DOS) of the system. The DOS becomes independent of energy in each of the subbands of a two-dimensional confined quantum well, resulting in a step wise accumulation of carriers as the Fermi level passes over the quantised states. Alternatively, in quantum wires (i.e., confined in one dimension) the DOS varies inversely with the square root of the energy from bottom of the subband, resulting in van Hove singularities. This alteration will affect the rate at which charges accumulate, change the quantum capacitance and impact effective gate control. Therefore, the threshold characteristics of lower dimensional systems are less dependent on the subband alignment and undergo a more pronounced turn-on behaviour. Additionally, the quantisation introduced by the confinement increases energy levels and results in a shift in the amount of voltage measured across solutions having different subbands that is proportional to the quantisation energy. The dimensional dependency of the DOS highlights the essential value of electrical engineering for the appropriate design and modeling of quantum semiconductor devices.

2.2 Energy Quantization and Carrier States

Energy Quantization increases due to a limited number of boundaries for the carrier wave function due to confinement. The Schrodinger Equation explains the electrons and holes are permitted within the energy and where they are able to exist. Based on the physical modeling described in [3], the physical structure and its associated states control that carriers

occupy the states, transfer between them, and can perform optical transitions. Quantum states have a direct impact the way that electrical currents flow and the threshold for electrical current to flow in a device, but carrier transfer happens, compared to continuous energy bands. Studies performed mathematically to predict [7] these discrete energy states are essential to the accurate simulation of a device. Minor deviations from the optimal electrostatic potential and/or geometry may lead to modifications in which the states are aligned/distributed for the carriers to occupy. As seen in Figure 4, the energy states for carriers resulting from confinement are quantized to show the quantization of energy and carrier state in structures can be represented, the formation of discrete subbands and the density of states properties.

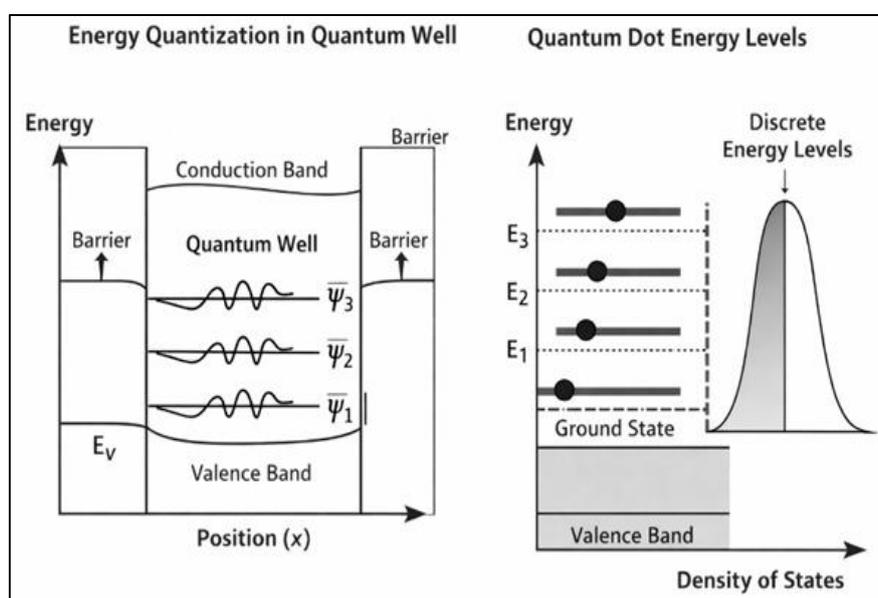


Figure 4. Representation of Band Structure of Low-Dimensional Semiconductor Structures

The interface between materials and the nature of electrostatics also affects the energy state of carriers. Atomically determined disorder and the interface surface roughness, as reported in [12], result in the localization of the wave function and consequently the size of the energy gap. As a result of this sensitivity, it is necessary for production techniques faces high manufacturing requirements and provide a purpose for using advanced modelling techniques that can directly resolve the quantum states of materials.

2.3 Quantum Transport and Tunneling

There are two separate categories of transportation: classical and quantum. In nanoscale systems, carriers travel as wave packets and exhibit phase dependence. One of the most

important transport mechanisms in a quantum device is called tunneling; it allows carriers to travel through impenetrable barriers.

The current review will focus on modeling quantum tunneling using the Wentzel-Kramer-Brillouin (WKB) approximation of transmission through a barrier. The probability of tunneling through a potential barrier is given as:

$$T(E) \approx \exp\left(2 \int_{x_1}^{x_2} \sqrt{\frac{2m^*}{\hbar^2} [V(x) - E]} dx\right) \quad (3)$$

m^* is the carrier effective mass of the carrier,

$V(x)$ is the potential barrier,

and x_1, x_2 are the classical turning points.

It is a semi-classical approximation that is computationally efficient and physically consistent describes the effects of tunneling in nanoscale semiconductor structures (especially smoothly varying potential barriers).

Tunnelling becomes increasingly essential as limitations are reduced, as indicated by the research in [7]. For an example, the use of tunnel field effect transistors and single electron circuits in machine design. When the mechanism of tunnelling can be controlled, then the devices can exhibit sub-threshold precision and low voltage activation. If tunneling is uncontrolled, it causes higher leakage current and reduces the device's isolation qualities.

The research conducted on experimental semiconductor devices has shown in [9] that tunnelling-induced leakage is a critical problem for ultra-scaled devices. Therefore, both material selection and barrier design are critical issues. Transport models will require current can be predicted accurately, which will require that tunnelling probabilities and wave function overlap, can be a part of the transport model. Classical mobility - based models can no longer be utilised in this domain.

2.4 Self-consistent Schrodinger Poisson Modelling

Developing a self-consistent analysis for quantum semiconductor devices will be challenging when carrier state issues and electrostatic potentials are properly handled. To

define a quantum state, use the Schrödinger equation, and solve the Poisson equation for induced charge or charge-induced potential. The equations mentioned above are connected together in a self-consistent way and need an iterative solution technique.

Numerous self-consistent Schrodinger-Poisson solvers have been discussed in [8], wherein the convergence of the algorithms used to determine the solution and stability of the numerical solution have been evaluated. Specifically, the authors indicate that errors in the computation process may increase from improper combining of the two equations and from poor spatial discretization, resulting in inaccurate behavior of the energy spectra. Thus, in order to produce an accurate analytical estimation of the carrier density within quantum materials, the study must be execute using proper numerical and analytical techniques.

The quantum mechanical equation of motion, i.e., the time-independent Schrodinger equation is useful in determining the quantum mechanical behaviour of charge carriers confined within semiconductor devices:

$$\left[-\frac{\hbar^2}{2m^*} \nabla^2 + V(r) \right] \psi_i(r) = E_i \psi_i(r) \quad (4)$$

In which, \hbar is the reduced Planck constant,

m^* is the carrier effective mass,

$V(r)$ is energy of the electrostatic potential,

$\psi_i(r)$ is the wave function and

E_i is the quantized energy levels.

The Poisson equation is used to solve to get electrostatic potential inside the device:

$$\nabla \cdot (\epsilon \nabla \phi(r)) = -\rho(r) \quad (5)$$

ϵ is the dielectric permittivity,

$\phi(r)$ is the electrostatic potential,

and $\rho(r)$ is the space charge density.

The carrier charge density is calculated out of the quantized states as:

$$\rho(\mathbf{r}) = q \sum_i |\psi_i(\mathbf{r})|^2 f(E_i) \quad (6)$$

q is the elementary charge

$f(E_i)$ is the Fermi-Dirac occupation function.

The equations are solved in an iterative manner in order to get self-consistency between quantum carrier states and electrostatic potential.

This paper presents a review of the different modeling frameworks provided in [10]. These modeling frameworks include various numerical methods used to help increased solver convergence, improve performance of the calculated solutions and provide designers with greater predictive capability about device parameters that will be used in their actual operating environments. At this time, self-consistent modeling has become a critical part of the design of quantum dots, junctionless devices and atomic transistors.

Developing the Schrodinger-Poisson model, that predicts semiconductors operate, requires a combination of theory, modeling, and production. It is important to use stabilization strategies in high bias and extreme tunneling regions of this model will have reduced numerical errors. There is one method for implementing possible reduction and adaptive filtering techniques to solve rapid oscillations caused by sudden charge redistributions. The second method is to generate lower bias states that will serve as the foundation for computing the solutions and the starting points for higher bias state solutions that are significantly more stable than the solutions itself. The third strategy for mesh refinement will utilize micro and adaptive meshes around barrier interfaces with large potential gradients and tunneling characteristics. Finally, theory conditions are imposed to ensure that charge can never be found at non-physical locations. In general, these stabilization methods provide added numerical stability to the mesh, remove the possibility for divergence and allow for reasonable convergence of the results for all operating conditions for quantum semiconductors.

2.5 Theory, Modeling and Production Interdependence

Quantum confinement explains the behavior of devices. However, atomic-level accuracy in manufacture is required to operate in real life. Thus, modeling accuracy has a significant connection to manufacturing variability in terms of variations in quantized energy levels caused by geometry or doping changes. This reliance demonstrates that simulation

development should be encouraged by nanotechnology enhancement with the aim to assure the device's high efficiency.

2.6 Thermal Effects and Temperature-Dependent Quantum Behavior

The importance of temperature in modern quantum semiconductor devices can't be highlighted. Specifically, increasing temperature causes carriers to occupy higher energy levels, which will lead to an increased probability that they will tunnel contributing to the leakage current and stability of the device being tested.

Experimental evidence of this connection is found in [21], states that thermal management is one of the major limiting factors for quantum devices with a size range close to the point at which quantum tunnelling will be used as the primary method of cooling to adequately control local heating. This will illustrate the connection between the thermal properties of a quantum device and the principles of quantum transport.

The results of reliability studies indicate that temperature changes have a direct connection to device yield variability both when producing and testing devices. Studies on cryogenic devices have shown high reproducibility and stability, while adding considerable complexity to system design. As a result, thermal conditions must be an essential element of consideration in prototyping both during experimentation and in end-use applications.

The Schrödinger-Poisson model represents the actual physical processes, but due to the complexity of solving these models using them to conduct large-scale explorations is inefficient and limits the scope of investigation. Conversely, machine learning models can be computed rapidly, but this advantage may result in reduced interpretability and extrapolation reliability. Therefore, the most reasonable path forward would be to use a combination of methods during the earliest stage of design and to use theory-based models to evaluate and verify designs as they become closer to being ready for production.

Table 1 contains a summary of the major distinctions between practical applications in larger quantum semiconductor device configurations, including operating environment, sensitivity to production models requirement.

Confinement geometry, material interfaces, and thermal conditions are important to the achieving confusion features in quantum semiconductor devices. Strong carrier localization is

usually observed in quantum dots and atom-based devices implications that higher coherence times can be achieved, but this technology must be operated at low temperature to overcome scattering by phonons. In quantum wells and quantum wires can be operated at room temperature in some applications, they suffer a high confusion rate because of increased carrier-phonon interactions and interface fluctuations. The single-electron and dopant-type devices have been demonstrated to be relatively robust in regard to coherence, despite their significant sensitivity to charge noise and thermal stimulation. In general, temperature increases accelerate the process of decoherence through phonon coupling, increasing of energy levels and the chance of tunneling. These thermal constraints effectively establish practical restrictions on the functioning of a device under temperature circumstances, requiring special focus on thermal management and material engineering in the design of quantum devices.

Table 1. Comparative Performance of Major Quantum Semiconductor Device Types

Device Type	Typical Operating Temperature	Production Tolerance	Modeling Complexity	Scalability Level
Quantum Wells	Room temperature - low	Moderate – thickness	Medium – confinement with reduced-order Schrödinger–Poisson models	High
Quantum Dots	low	Low – strong sensitivity to size, shape, and interface roughness	High – full 3D confinement	Medium – scalable
Quantum Wires	Low-moderate	Low – cross-sectional uniformity is difficult to maintain	Strongly affected by edge scattering and quantization	Low to Medium – integration
Single-Electron Devices	Cryogenic	Very Low atomic-scale	Very High requires	Low – large scale integration
Tunnel FETs	Room temperature	Moderate to Low	High – tunneling probability	Medium to High – CMOS-compatible variants
Atom-Based / Dopant-Based Devices	Cryogenic - low	Extremely Low –	Very High	Very Low

3. Quantum Semiconductor Device Modeling and Simulation

The development of quantum semiconductor devices is mainly based on modeling and simulation. Trial and error methods of experimentation are expensive and unfeasible as the size of the device is reduced. The correct models are needed to forecast the behavior of devices prior to manufacturing. Compact classical models cannot be applied in quantum regions. New models will have to represent confinement, tunneling, electrostatics and variability in the same model. More recent reviews provided in [12], indicate that quantum device modeling has developed into a more hybrid numerical and data-driven design compared to traditional theory-based formulations. This evolution indicates the increased complexity of device development and operating circumstances. Modeling accuracy discontinues effects productivity, yield and dependability.

3.1 Modeling Approaches Based on Theory

Quantum semiconductor simulation is still based on theory-based modeling. These models are based on initial-principles models or semi-classical models developed based on quantum mechanics and solid-state physics. The theoretical model presented in [13] is the derivation of carrier states, potential profiles and transport mechanisms based on basic equations.

Schrodinger based formulations on a nanoscale are evaluated to obtain quantized energy levels and wave functions. Electrostatic solvers are combined with these results to obtain the profile of charge and potential profiles. The transport is frequently described by quantum ballistic or non-equilibrium Green functions techniques [14]. These models are accurate physically but demanding in terms of computing. Models based on theory is required to explain the device behavior. It fails to scale when there are many parameters. This issue encourages the formulation of more effective modeling schemes that maintain physical integrity of the model but are low cost to compute.

Although theoretical simulations using theory models suggest high confinement and tunneling, practical implementation has shown that there are interface traps, phonon scattering and disorder caused by production causes a decline in performance. This difference between theory and experiment is a significant challenge in quantum device design.

Quantum modeling techniques are theory-based various complexities modeled computationally. Self-consistent solvers (Schrodinger-Poisson solvers) have self-consistent and have a time expense that scales like the size of the mesh and the time to compute the eigenvalues. Therefore, to diagnosis the full matrix, the cost of the computation is $O(N^3)$ where N is the size of the mesh separated. The expense of using non-equilibrium Green functions quantum transport models will further increase the time expense per evaluation. Semi-classical approximations and reduced order quantum corrections also provide moderately accurate results with less computational intensity when compared to the machine learning-assisted substitute models. Alternatively, when trained the machine learning-based substitute models provide inferential results in virtually constant time, resulting in a considerable decrease in the amount of time required to analyze enormous design spaces. The complexity of training and dependability of the training dataset are also critical factors. Therefore, this highlights the tradeoff between physical and computational efficiencies in modeling quantum devices.

3.2 Numerical Simulation and Convergence Challenges

Numerical implementation is a critical aspect of quantum device modeling. Discretization and iteration using coupled quantum equations is an important part of this process. In their study, Lach et al [15] found that there are many convergence issues associated with self-consistent Schrodinger Poisson solvers. These convergence issues lead to the potential for obtaining unstable solutions if the initial conditions or the mesh size are not optimal.

There is a high correlation between mesh resolution [16] and the accuracy of the energy packing level. Fine meshes will lead to accurate values, but will also increase the time it takes to perform calculations. Therefore, it is often necessary to use adaptive in meshing methods. The convergence behaviour of these methods will also depend on the boundary conditions chosen to model the interfaces of the physical devices.

There are more challenges provided by transport simulations. Quantum transport equations are complex matrix equations and integrations of energy. Numerical stability is a sensitive parameter with temperature, bias conditions and material parameters. These issues are necessary to achieve the reliable simulation results and reproducible results.

3.3 Modelling of Devices with the Help of Machine-Learning

Recent research demonstrates an increasing interest in the fusion of traditional theory models and new machine learning techniques such as data science. For example, systems model represented in [6] demonstrates how machine learning can enhance forecast accuracy and the developing run time or executing simulations from valid physical data.

According to the authors referenced in [17], the use of substitute models based on learning could be potentially used to create models with complex, high-dimensional response surfaces prior to performing optimization on designs. Although the physical model exists, these substitute models can decrease the time required to obtain an approximate estimate of different characteristics/properties of a large number of designs based on the physical characteristics of the designs of interest at the same time as developing or optimizing those designs.

All models must be created and trained accurately to a high level of integrity so that the laws of mass/angular/momentum conservation and the appropriate forms of energy conservation are valued. For example, as new or improved physical constraints for the primary model frameworks are identified or represented, hybrid prediction methods such as machine learning based framework and physical constraints will provide results which are predictive, accuracy levels, and also easily comprehensible and execute efficiently.

The simulation of quantum semiconductor devices has an inherent trade-off between the amount of computer resources consumed and the accuracy of the simulation of real-world device effects such as confinement, tunnelling and quantum transport, through the use of physical models based on real-time theory (for example, self-consistent Schrödinger/Pneumann methods, NEGF method, etc.). However, solving these models will often require substantial amounts of computational resources because of the requirement to solve eigenvalue problems and perform matrix operations.

Physical models usually suitable for the verification or analysis of a device. On the other hand, substitute or reduced-order models (with machine learning enhancements) will allow the simulation of the same device design space at reduced computer resource requirements than physical models and therefore support the evaluation of huge design space. However, substitute/reduced-order models produce approximate solutions and have limitations when it comes to the interpretability/reliability of modeling their results. In general, the model

will be selected based on some combination of trade-offs between accuracy, computer resource utilization and the overall design exploration objectives defined for the project.

Recent research has shown that a number of machine learning architectures have performed well to quantum semiconductor devices modeling. Deep feedforward and physics-informed neural networks (PINNs) are popular neural networks are used to approximate the nonlinear characteristics of a device. Gaussian process regression has demonstrated a high level of uncertainty-aware substitute modeling and support vector machines provide high quality performance in parameter sensitivity analysis. Also, convolutional neural networks have been considered to extract structure-dependent features in nanoscale devices. These models can be used to predict large design space much faster, but their accuracy is limited by the quality of training data and physical consistency limits.

3.4 Yield Aware and Variability Sensitive Modeling

One of the major problems in the production of quantum semiconductor devices is their variability. Minor changes in geometry, doping or interface quality may cause significant performance changes. As the study of yield diagnosis presented in [18] shows, the traditional nominal modeling cannot produce the model that can reflect these effects.

Yield-aware simulation applies statistical variations to the simulation processes. The performance is tested by sampling parameter distributions. The sensitivity analysis determines major sources of variability. These approaches make it possible to identify important steps in the process early. The detailed discussion in [19] also highlights the variability modeling is required to convert laboratory prototypes into technologies that can be produced. In the absence of yield-sensitive simulation, it lacks the feasible to scale quantum devices to large arrays.

3.5 Integration with Electronic Design Automation Frameworks

It is necessary to provide electronic design automation tools with a description of the devices and they are built to make quantum devices useable in practice. These models of devices can increase the accuracy of circuit-level simulation, as noted in [20]. As a result, electronic designers would be able to execute an electronically designed system at the system level while expecting realistic device performance from the designed system normally occur in a design utilizing standard-type devices.

Compact models based on quantum simulations estimate the impact of quantum effects; therefore, they are generally not computationally expensive. The numerical evaluations need to be performed to confirm the results of compact models to ensure their validity.

As indicated in the modeling system of [21], the future steps in the design process will be accomplished using a multi-level modeling approach. The compact models will be used in combination with precise quantum simulations allowing large-scale analyses of a circuit and system to take place based on these models. In order to help the connections between quantum device physics and the performance of real-world electronic systems.

In the quantum semiconductor field, there are various types of device structures and methods of fabricating devices. It is within the scope of this work to provide a detailed description of all of these items; instead, to maintain speed and clarity, the review work has compiled a summary of the largest quantum device forms and methods of production provided in the literature in Table 2.

Table 2. Quantum Semiconductor Device Architectures and Production Approaches

Category	Device Type / Approach	Key Observations from Literature	Main Challenges
Quantum confinement devices	Quantum wells and quantum dots	[14] show strong energy quantization and size-dependent behavior	Sensitivity to size variation
Atom-based devices	Atomic-scale quantum dots	[13] and [12] demonstrate stable confined states with precise dopant placement	Production complexity
Junction-less devices	Ultra-scaled FET structures	[9] indicates improved electrostatic control	Variability and leakage
Optoelectronic quantum devices	Quantum dot energy devices	[19] [22] reports enhanced optical absorption	Long-term stability

The design and production of devices, their stable operation involves the precision of the modeling, diagnostic capabilities and thermal control. These factors directly affect the output and productivity of the real-life applications. A comparative overview of the modeling, diagnostics and thermal considerations is provided in table 3.

Table 3. Modeling, Diagnostics and Thermal Considerations in Quantum Semiconductor Devices

Aspect	Focus Area	Insights from Literature	Limitations Identified
Device modeling	Theory-based and hybrid models	[1] and [6] report improved prediction accuracy	High computational cost
Numerical stability	Solver convergence	[8] highlights convergence sensitivity in Schrödinger–Poisson solvers	Stability at high bias
Yield diagnostics	Fault identification	[4] and [20] show early detection improves reliability	Limited in-situ monitoring
Thermal behavior	Heat dissipation and cooling	[21] indicate tunneling-assisted cooling can reduce local heating	System complexity

The multiple new applications are under consideration related to quantum semiconductor devices and the long-term sustainability and scalability remains a significant issue. These are some of the factors that influence future research directions. Table 4 presents the important applications and forecasted trends in the recent studies.

Table 4. Applications, Sustainability and Future Trends of Quantum Semiconductor Devices

Aspect	Current Direction	Reported Findings	Future Outlook
Computing and sensing	Quantum hardware platforms	Experimental demonstrations in [11] and [17] show feasibility of semiconductor-based qubits	Scalable architectures
Energy applications	Quantum dot energy devices	Results in [19] indicate improved efficiency due to quantum effects	Device integration
Material sustainability	Semiconductor recovery	The study in [18] highlights resource and lifecycle concerns	Sustainable materials
Technology roadmap	Atomic-scale integration	Roadmap analysis in [12] outlines long-term device scaling paths	Industry adoption

4. Findings

In this paper, the recent advances in quantum semiconductor devices were reviewed. Basic quantum theory, manufacturing methods, modelling devices and dependability were discussed. This review found that quantum confinement, tunnelling and energy quantization have a significant impact on device behavior at the nanoscale. It also explains better modeling and accurate manufacturing are required for long-term operating stability. The comparison

tables summarized existing device architecture, modelling and application developments reported in the literature.

5. Challenges

Scalability and large-scale production are the two major challenges to the practical application of quantum semiconductor devices. This is one of the major challenges that proves challenging to integrate into traditional CMOS manufacturing processes. Although several quantum device concepts have been demonstrated to operate successfully in the laboratory, they must be coordinated with traditional silicon-based process flows, existing materials, temperature budgets and lithographic procedures. Non-standard CMOS process variations frequently increase process cost and manufacturability. Another issue is that quantum devices depend on feature sizes and dopant location near atomic scale. The minor changes in device design lead to significant results in confinement patterns and tunnelling probabilities provide unreliable device behavior. The increased sensitivity impact significant production trade-off between device size and manufacturing consistency. The reduced dimension and effective device per wafer leads to the differences in interface errors, line-edge quality and random dopant variations. Furthermore, the quantum semiconductor architecture and design systems required defect-tolerant can allow sustainable performance in manufacture-related defects. These methods can involve redundancy, adaptive calibration and error-tolerant circuit design connects the scalable industrial manufacturing and laboratory models.

6. Conclusion

Quantum semiconductor devices have an immense effect on the future of electronics. Numerous physical and technological challenges remain with significant advancement has been achieved. In this review, the study provides an overview of the most recent developments and major flaws. It should also be valuable for researchers and engineers focusing on dependable and scalable quantum semiconductor devices. In future, the system will focus on manufacturing accuracy and dependability in the industrial regions. It is required to improve thermal management methods of stable electronics. The demand for scalable modelling system can handle huge number of devices. It is required before the quantum semiconductor technologies use real-time applications

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