http://www.doi.org/10.62341/rfoh2612

Received	2025/11/27	تم استلام الورقة العلمية في
Accepted	2025/12/18	تم قبول الورقة العلمية في
Published	2025/12/19	تم نشر الورقة العلمية في

Self-consistent Schrödinger-Poisson Study of AlAs Barrier Thickness Effects in GaAs/AlAs Resonant Tunneling Diode

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Abstract

This study examines the impact of quantum barrier thickness on the current–voltage (I–V) characteristics of a Resonant Tunneling Diode (RTD). Electron transport across a double-barrier GaAs/AlAs heterostructure was modeled using a self-consistent Schrödinger–Poisson simulation. By varying the barrier thickness from 2 nm to 6 nm, tunneling probability, resonance peak position, and Peak-to-Valley Current Ratio (PVCR) were analyzed. Results show that thicker barriers shift the resonance peak to higher bias voltages and reduce tunneling current due to decreased transmission probability. These findings highlight the critical role of barrier geometry in optimizing RTD performance for low-power and high-frequency nanoelectronics applications.

Keywords: RTD; quantum barrier thickness; Schrödinger–Poisson simulation; I–V characteristics; tunneling probability; GaAs/AlAs heterostructure.

http://www.doi.org/10.62341/rfoh2612

دراسة شرودنجر بويسون ذاتية الاتساق لتأثيرات سمك حاجز AlAs في ثنائي نفق الرنينGaAs/AlAs

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الملخص

تبحث هذه الدراسة في كيفية تأثر خصائص التيار-الجهد (I-V) للثنائي النفق الرنيني (RTD)بسمك الحاجز الكمي. نُمذِجَت عملية نقل الإلكترونات عبر بنية غير متجانسة ثنائية الحاجز من GaAs/AlAs باستخدام محاكاة شرودنجر-بويسون ذاتية الاتساق. ودُرِسَ احتمال النفق، وموضع ذروة الرنين، ونسبة تيار الذروة إلى الوادي (PVCR) بتغيير سُمك الحاجز من 2 نانومتر إلى 6 نانومتر. وتُظهِر النتائج أن زيادة سُمك الحاجز تدفع ذروة الرنين نحو جهد انحياز أعلى، وتُقلِّل تيار النفق نتيجةً لانخفاض احتمالية النقل. وتُبيّن هذه النتائج أهمية هندسة الحاجز في تعظيم أداء RTD في تطبيقات الإلكترونيات النانوية منخفضة الطاقة وعالية التردد.

الكلمات المفتاحية: (RTD) سُمك الحاجز الكموي؛ محاكاة شرودنجر-بويسون؛ خصائصI-V ؛ احتمال النفق؛ بنية غير متجانسة من.GaAs/AlAs .

1. Introduction

Terahertz (THz) emission sources have been extensively researched due to applications in medical imaging, radar, security, and communication technologies [1,2]. Resonant Tunneling Diodes (RTDs) are suitable THz sources because of their high cutoff frequency and superior power output [3,4]. Gallium nitride (GaN) terahertz oscillators are particularly efficient due to their wide

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bandgap, strong carrier mobility, high electron peak velocity, thermal stability, and high electron saturation rate [5,6].

The maximum theoretical operating frequency of RTD-based oscillators depends on the peak voltage-to-valley ratio (PVR), influencing output power [7]. Enhancing peak current, reducing valley voltage, and improving PVR are key goals in recent GaN-based RTD research. RTDs exhibit negative differential resistance (NDR), enabling ultrafast oscillators and switches in microwave and terahertz circuits [8]. Structurally, a quantum well lies between two potential barriers in a GaAs/AlAs RTD [9]. Electrons tunnel through both barriers when the applied bias matches the discrete energy levels in the quantum well, producing a pronounced current peak followed by an NDR region [10]. Barrier and well geometry significantly influence these I-V features [11].

2. Methodology and Theoretical Model

The RTD structure consists of a 5 nm GaAs quantum well and two AlAs barriers with thicknesses ranging from 2 nm to 6 nm. The conduction band offset between GaAs and AlAs is assumed to be 0.5 eV. Electron transport was modeled using a self-consistent Schrödinger–Poisson solver to determine potential profiles and subband energies under applied bias. The one-dimensional Schrödinger equation for electrons in the conduction band is:

$$E\phi(z) = V(z)\ \phi\ (z) + \frac{dy^2}{2_{dx}}\ \frac{h^2}{2m*(z)} \quad \text{.........................} 1$$

Where m*(z) is the position-dependent effective mass and V(z) is the conduction band potential profile. The current density J was calculated using the Tsu–Esaki formula:

$$f_2\ (E)dE - T(E,V)f_1 \int \frac{e}{2\Pi h^2} = J(V) \quad \text{.........................} 2$$

3. Simulation Framework

The GaAs/AlAs RTD was modeled as a one-dimensional quantum device along the growth direction. Material parameters (effective

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mass, dielectric constant, bandgap, conduction-band offset) were taken from established literature. Simulations were performed using nextnano++ with a non-uniform finite-difference mesh refined at interfaces, quantum well, and barriers. The Schrödinger equation solved for bound and quasi-bound states under applied bias, while the Poisson equation determined electrostatic potential. Self-consistency was achieved iteratively until potential differences were below 1×10^{-6} eV. Boundary conditions fixed Fermi levels at contacts and applied external bias. Electron density from sub band wavefunctions was fed back into the Poisson solver. Simulations were carried out at 300 K unless specified. Validation was done by comparing simulated resonance energy levels and I-V characteristics with experimental and theoretical results, and cross-checked with MATLAB scripts.

The conduction band profile and transmission probability for various barrier thicknesses are shown in Figure 1. Increasing barrier thickness decreases tunneling probability and shifts resonance to higher bias voltages. The band gap (Eg) varies with thickness due to quantum confinement effects, with smaller thickness producing stronger confinement and larger Eg, and larger thickness producing weaker confinement and smaller Eg.

4. Effect of Barrier Thickness

Quantum confinement causes significant changes in electronic and optical properties. At 2 nm thickness, strong confinement separates energy levels, increases Eg, reduces conductivity, and enhances non-metallic behavior. At 6 nm thickness, confinement weakens, energy levels converge, Eg decreases, and conductivity improves.

Experimentally, thin films of 2–6 nm were prepared, optical absorption measured via UV-Vis spectroscopy, and Eg extracted using Tauc plots. Results confirm that Eg decreases with increasing thickness, enhancing electrical conductivity and altering optical properties.

This is all due to quantum confinement, which dominates when matter becomes extremely thin as shown in Figure 1.

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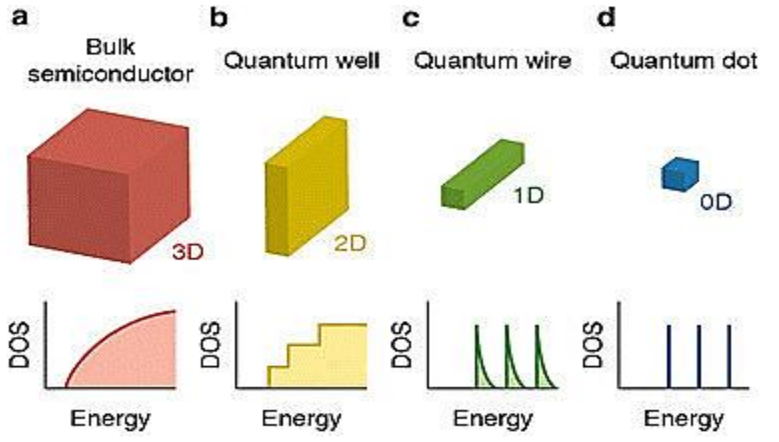

Figure 1: Schematic illustration of energy gap changes due to quantum confinement [12]

5. I–V Characteristics

Computed I–V characteristics are shown in Figure 2.

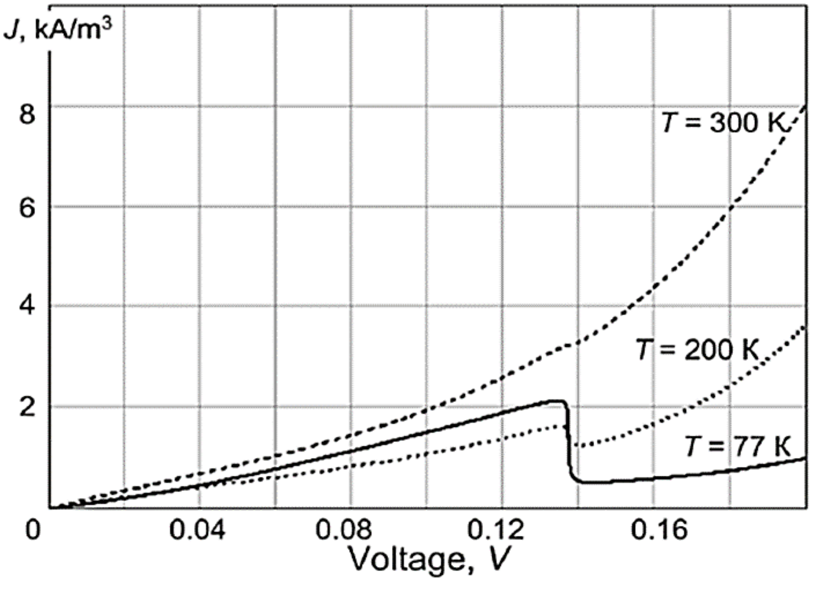

Figure (2). The calculated I-V characteristics [12].

For a 2 nm barrier, resonance occurs at 0.18 V with a peak current of 8.3 kA/cm². Increasing barrier thickness to 6 nm shifts resonance to 0.27 V and decreases peak current to 2.1 kA/cm². PVCR decreases from 6.2 to 2.9, indicating reduced NDR with thicker

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barriers. The tunneling current depends exponentially on barrier width:

$$\sqrt{\frac{2m*(V_0-E)}{h^2}}=e^{-2kd},\ k\ \alpha\ T \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \; 3$$

Where V0 is the barrier height and d is the barrier thickness.

6. Discussion

Thinner barriers enhance coupling between the quantum well and contacts, increasing tunneling current. Excessive thinning reduces PVCR and increases leakage. Thicker barriers increase confinement but reduce coupling, shifting resonance to higher voltages and decreasing current density. Optimal barrier thickness (typically 3–4 nm for GaAs/AlAs RTDs) balances high current density with sufficient NDR for high-frequency applications.

7. Conclusion

This paper investigated the effect of barrier thickness in a resonant tunneling diode (RTD) on its current-voltage (I-V) characteristics. The study analyzed how quantum tunneling behavior changes with increasing or decreasing the thickness of the quantum barrier—typically made of materials such as GaAs/AlAs. The results showed that increasing the barrier thickness reduces the probability of tunneling, leading to a decrease in peak current and a shift in resonant voltage due to changes in the quantized energy levels within the quantum well. Furthermore, thicker barriers improve the peak-to-valley current ratio (PVCR) by reducing the valley current, although they also decrease the overall device current. The study concludes that precise control of barrier thickness is crucial for tuning the performance of the resonant tunneling diode, influencing the shape of the resonant voltage (I-V) curve, and maximizing efficiency in high-frequency applications.

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