

Self-consistent analysis of the miniband structures in superlattice quantum wires

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Abstract

The miniband and minigap structures of the lateral superlattice quantum wires in grid-inserted quantum well are analyzed by using a self-consistent finite-element method with a periodic boundary condition. Conduction band diagram and the mobile charge concentration as well as the energy dispersion relation are self-consistently analyzed. It is shown that even a few monolayers of AlAs at the center of the GaAs quantum well can create a minigap greater than 10 meV resulting in anisotropic carrier transport.

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1. Introduction

The superlattice quantum wires embedded in the two-dimensional electron gas (DEG) layer or charged layers have been interesting research subjects due to their anisotropic transport properties which can be utilized as ballistic rectifiers [1–2]. One example is the in-plane superlattice consisting of a grid-inserted quantum well (GIQW) structure [3]. The structure is the same as the typical quantum well structure except that a periodic fractional layer is inserted in the middle of the quantum well layer. This grid is formed by depositing a fractional monolayer of AlAs on the vicinal GaAs surface [4]. The lateral step width, D , depends on the tilt angle of the surface with respect to the horizontal axis. For example, D is 16 nm when the tilt angle is 1° . The insertion of the grid in the quantum well layer would bring forth minibands and minigaps.

In this paper, such miniband and minigap structures in GIQW superlattice quantum wires are analyzed by using a self-consistent finite-element method in conjunction with a periodic boundary condition. Conduction band diagram and the mobile charge concentration are self-consistently analyzed as well as the energy dispersion relation with

respect to the wave vector along the lateral direction to optimize the minigap structures.

It has been shown that even a few monolayers of AlAs at the center of the GaAs quantum well can create a minigap greater than 10 meV. Finally the anisotropic transport properties of those structures are investigated for sign-reversed ballistic rectifiers.

2. Miniband characterization

Due to the quantization of the electron wavefunctions in the transport regions, full understanding of the conduction properties of these structures requires the self-consistent solution of both Poisson and Schrödinger equations. A conventional approach to this problem is to use the finite-difference method [5] or the finite-element method. Since the charge distribution is closely related to the electrostatic potential, the governing Poisson equation should be iterated until the charge and the electrostatic potential are self-consistent. However, either direct iteration converges slowly or even fails to in some cases. To guarantee and accelerate the convergence, the Newton–Raphson method has been used in the earlier heterostructure analyses [6]. The same technique can be also applied to the finite-element method. To do so, the charge concentration is expanded to the first order Taylor series as:

$$\nabla \cdot (\epsilon \nabla \Phi) + \rho_0 + \frac{\partial \rho}{\partial \Phi} \Big|_0 (\Phi - \Phi_0) = 0 \quad (1)$$

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where ρ_0 and Φ_0 are the values after n iterations, and ρ and Φ are the values after $(n+1)$ iterations. ε is the dielectric constant. The corresponding Lagrangian functional can be evaluated by integration by parts, which leads to

$$J = \int_{\Omega} \left[\frac{1}{2} \varepsilon (\nabla \Phi)^2 - \rho_0 \Phi - \frac{\partial \rho}{\partial \Phi} \left|_0 \left(\frac{1}{2} \Phi^2 - \Phi_0 \Phi \right) \right] d\Omega \quad (2)$$

where Ω is the cross-sectional area of interest. This new scheme greatly reduces the convergence speed [7] compared to the conventional FDM or FEM.

A schematic diagram of the one-dimensional electron transport in the split gate electron waveguide [5] is shown in Fig. 1. The 1DEG is formed by applying V_g on the Schottky gates, and the electrons are injected through the ohmic contacts by applying V_{ds} . The cross-sectional geometry of the 1DEG formed by the split gate is shown in Fig. 2, where the 1DEG region consists of the grid inserted quantum well (GIQW) structures. The specific profile of the cross-sectional layer analyzed [3] is as follows: The top layer is 10 nm GaAs cap layer and the second layer is 88 nm-thick $\text{Al}_{0.5}\text{Ga}_{0.5}\text{As}$. The doping layer is located at 64 nm below the interface within the $\text{Al}_{0.5}\text{Ga}_{0.5}\text{As}$ layer and the doping concentration is $7 \times 10^{18}/\text{cm}^3$. The quantum well is 13 nm-thick GaAs. The monolayer AlAs grid is inserted at the middle of the quantum well and covers half of the step width, where $D=32$ nm. The bottom substrate is $\text{Al}_{0.21}\text{Ga}_{0.79}\text{As}$.

The lateral superlattice is modeled as a periodic potential profile, thus the periodic boundary conditions are applied to solve for Poisson and Schrödinger equations. Fig. 3 shows the self-consistent solutions of the conduction band diagram and the mobile charge profile along the vertical axis passing through the center of the AlAs grid at $V_g=0$ V.

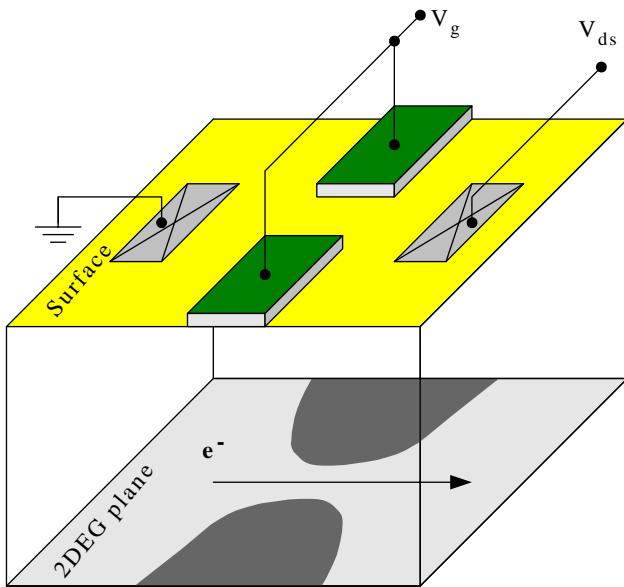


Fig. 1. Schematic diagram of the 1D electron transport in the split-gate electron waveguide.

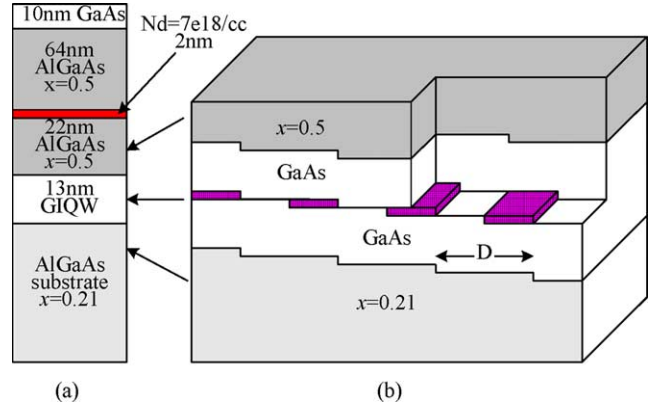


Fig. 2. Grid-inserted quantum well (GIQW) structure. (a) The cross-sectional layer profile. x denotes the Al composition of each AlGaAs layer. (b) The schematic diagram of the GIQW structure.

The conduction band minimum at the quantum well is -72 meV, and the peak carrier concentration is $1.57 \times 10^{17}/\text{cm}^3$. Due to the AlAs grid, the charge concentration has a dip at the center of the quantum well. Since the position of the AlAs fractional monolayer coincides with the peak of the electron wave functions in the quantum well, the effect of the perturbation by a monolayer becomes maximized. Hence even one monolayer can create significant miniband gaps. Fig. 4 shows the electron energy dispersions of the grid-inserted quantum well with respect to the Bloch wavenumber along the lateral direction in the range of 0 to π/D . The solid lines are for the in-plane lateral superlattice of a GaAs/AlAs monolayer at the center of the quantum well. The energy spacing between the two lowest subbands constitutes the miniband gap. When the lateral superlattice is replaced with the laterally uniform $\text{Al}_{0.5}\text{Ga}_{0.5}\text{As}$ digital alloy, the miniband gaps disappear as shown by the dotted lines.

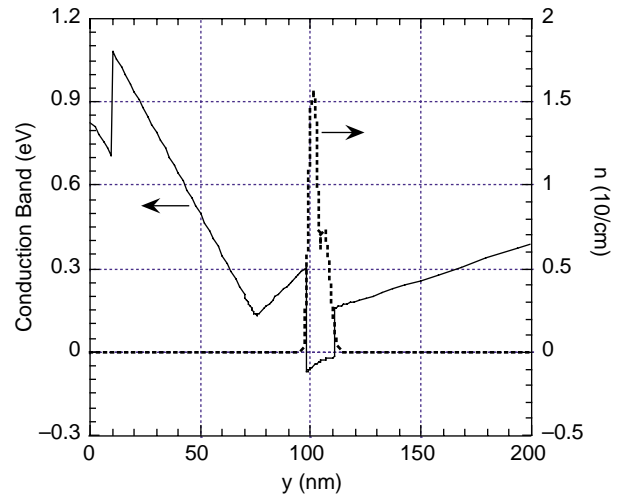


Fig. 3. Conduction band diagram (solid line) and the mobile charge concentration (dotted line) along the y -axis in the grid-inserted quantum well structure. In the center of the quantum well, the charge concentration has a dip due to the AlAs grid.

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