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Electrical transport engineering of semiconductor superlattice structures

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ABSTRACT

We investigate the influence of doping concentration on band structures of electrons and electrical transmission in a typical aperiodic semiconductor superlattice consisting of quantum well and barrier layers, theoretically. For this purpose, we assume that each unit cell of the superlattice contains alternately two types of material GaAs (as a well) and GaAlAs (as a barrier) with six sublayers of two materials. Our calculations are based on the generalized Kronig–Penny (KP) model and the transfer matrix method within the framework of the parabolic conductance band effective mass approximation in the coherent regime. This model reduces the numerical calculation time and enables us to use the transfer matrix method to investigate transport in the superlattices. We show that by varying the doping concentration and geometrical parameters, one can easily block the transmission of the electrons. The numerical results may be useful in designing of nanoenergy filter devices.

1. Introduction

In recent decades, the theoretical and the experimental researches on multilayer and heterostructures of mesoscopic and nanoscopic dimensions have been attracted a great deal of interest in the field of developing electronics since the pioneering works of Esaki and Tsu [1,2]. This is due to discovery of the nanofabrication techniques in materials science [3–6] and semiconductor superlattices growth [1,7]. A superlattice structure contains a periodic or aperiodic structure of repeating quantum wells and barriers which affects the conditions for charges to flow through the structure. The semiconductor supperlattice and heterostructures are of interest not only for their device applications but also for the fundamental physical phenomena they exhibit due to their material properties and low confined dimension. These structures can be produced using various techniques, but the most common of them are the molecular-beam epitaxy (MBE) and the metal-organic chemical vapor deposition (CVD) [7].

Due to the ability to change energy band structure and lattice parameters in III–V semiconductor compounds, they have received considerable attention for various semiconductor applications in designing superlattices and multilayers. According to this, the special optical and electrical properties of superlattices lead to their possible applications as new devices for example analogous device based on quantum well structure fabricated from GaAs sandwiched between two $Ga_{1-c}Al_cAs$ barriers with the doping concentration, c [8,9]. This device could handle frequencies up to 2.5 THz giving possibility to work at millimeter and submillimeter wave length and electron energy filter because the electronic responses of such devices can be tailored by varying the composition and thicknesses of these layers [10,11].

In order to understand the features exhibited in the electronic characteristics and optical spectra of superlattices, it is essential to calculate their electronic band structure. A number of theoretical methods have been applied to the study of such calculations. One method is the tight-binding approximation which is able to include the contributions from the Brillouin zone of the bulk materials in calculating the zero-folded bands in superlattices [12,13]. Moreover, we can study the band structure of superlattices using the envelope function approximation which can be explained by the Bloch theorem [14,15]. Another one is the first principles calculations of superlattice structure. Although this method, which uses quantum theory for electrons by including many-body interactions, can be more accurate than calculations based on the KP model, the computations involved is very intensive and limited to a few unit cells [16].

In this paper, we apply the second method with proper boundary conditions, and investigate the changes in dispersion energy and transmission coefficient of electrons in the semiconductor superlattices with each unit cell containing several sublayers of two materials of GaAs and $Ga_{1-c}Al_cAs$. Regarding the effect of resonance tunneling of electrons, we have new physics for our problem and solve it in the frame of Kronig–Penny (KP) model [17] and transfer matrix (TM) method which enables us to

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calculate band structure using Bloch theorem. This model reduces the numerical calculation time and enables us to use the transfer matrix method to investigate transport in the considered superlattices.

The paper is organized as follows. After a brief overview of the periodic and aperiodic semiconductor superlattice (Section 1), we will describe, in Section 2, the GaAs/$Ga_{1-c}Al_cAs$ superlattice and the model to calculate band structure and electrical transmission, briefly. In Section 3, we discuss on the numerical results of the effect of doping concentration, c, on the transport properties in the aperiodic semiconductor superlattice. The last section of the paper is devoted to the discussion and conclusion of our findings.

2. Theoretical model and formalism

In this section, we investigate the electron band structure and electrical transmission properties in a type of superlattice structure based on III–V semiconductor materials by including different doping concentrations. The heterostructure superlattice (composed of N unit cells) formed by a sequence of semiconductor materials, GaAs (as a quantum well) and $Ga_{1-c}Al_cAs$ (as a barrier) layers, in which each unit cell contains m layers with different thicknesses as shown in Fig. 1.

Based on the parabolic conductance band effective mass approximation, the longitudinal part of the one-electron Hamiltonian can be written as

$$H_z = -\frac{\hbar^2}{2m_j^*}\frac{d^2}{dz^2} + U_j(c), \tag{1}$$

where m_j^* is the hole effective mass in the jth layer and is taken as $m_w^* = 0.067m_0$ and $m_b^* = (0.067+0.088c)m_0$ for the well and barrier materials, respectively, where m_0 is the free-electron mass [18]. Also, $U_j(c) = E_F + \phi_j(c)$ where E_F is the Fermi energy in the GaAs layer, measured from the edges of conductance band in this layer, and ϕ is the doping layer barrier height measured from the Fermi levels.

The Schrödinger equation for a low biased barrier layer can be simplified by a coordinate transformation whose solution is a linear combination of the exponent functions. Considering all regions of junction in the nth unit cell, the eigenfunctions of the Hamiltonian (1) with eigenvalue E_z have the following forms:

$$\psi_j(n,z) = A_j(n)\exp[ik_j(n)z] + B_j(n)\exp[-ik_j(n)z], \tag{2}$$

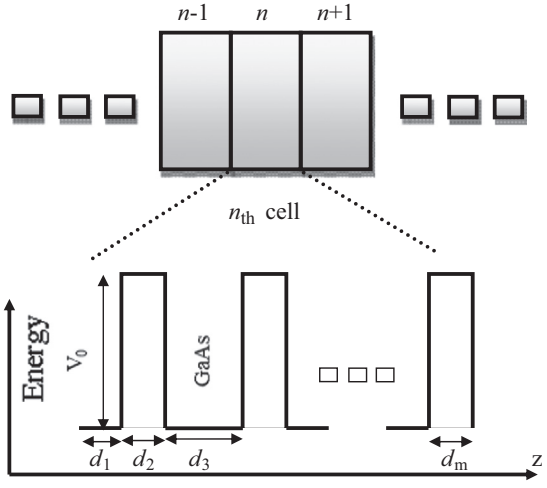

Fig. 1. Schematic representation of the heterostructure superlattice with each unit cell contains alternately two types of material GaAs (as a well) and GaAlAs (as a barrier) with m sublayers of two materials. V_0 is the barrier height which depends on the doping concentration.

where

$$\frac{\hbar^2 k_j^2}{2m_j^*} = \begin{cases} E_z, & j \in \text{well layer}, \\ E_z - V_0(c), & j \in \text{barrier layer}, \end{cases} \tag{3}$$

are the carrier wave vectors along the z-axis. The coefficients A_j and B_j are constants to be determined from the boundary conditions. Also, the potential barrier height measured from the Fermi level is assumed according to Ref. [18] as $V_0(c) = 0.65(1.36c + 0.22c^2)$. The considered system has translation asymmetry in the direction perpendicular to the growing direction z. Therefore, the transverse momentum $\mathbf{k}_\parallel$ is omitted from the above notations, namely, the summation over $\mathbf{k}_\parallel$ is carried out in our calculations.

The boundary conditions such that the wave functions and their first derivatives are matched at the interface between the quantum well and the barrier materials in the nth unit cell are

$$\begin{cases} \psi_w(z)|_{z_j} = \psi_b(z)|_{z_j}, \\ \dfrac{1}{m_w^*}\dfrac{d\psi_w(z)}{dz}\Big|_{z_j} = \dfrac{1}{m_b^*}\dfrac{d\psi_b(z)}{dz}\Big|_{z_j}, \end{cases} \tag{4}$$

where z_j is the position of the interface between jth and $(j+1)$ th layers. Upon applying the boundary conditions, we obtain a matrix formula that connects the coefficients $A_j(n)$ and $B_j(n)$ with the coefficients $A_{j+1}(n)$ and $B_{j+1}(n)$ as follows:

$$\begin{pmatrix} A_j(n) \\ B_j(n) \end{pmatrix} = \underbrace{\begin{pmatrix} M_{11}(n,j) & M_{12}(n,j) \\ M_{21}(n,j) & M_{22}(n,j) \end{pmatrix}}_{\mathbf{M}(n,j)} \begin{pmatrix} A_{j+1}(n) \\ B_{j+1}(n) \end{pmatrix}. \tag{5}$$

The total transfer matrix of each unit cell in the superlattice creates a recurrent equation as $\mathbf{M}(n) = \prod_{j=1}^{m}\mathbf{M}(n,j)$, where m is the number of layers in the nth unit cell. Therefore, the total transfer matrix of the system with N unit cells is given by $\mathbf{M}_{total} = \prod_{n=1}^{N}\mathbf{M}(n)$. Assuming the electron is incident from the left region (GaAs), only a transmitted wave exists in the right hand side of the superlattice (also GaAs), that is, $B_1(N+1) = 0$, and the transmission coefficient (TC) of the electron, which is defined as the ratio of the transmitted flux to the incident flux, can be written as [19–21]

$$\mathrm{TC}(E) = \left[\frac{1}{M_{total}(11)}\right]^2. \tag{6}$$

In order to calculate the band structure, we consider an infinite superlattice in which the coefficients of the wave functions in the different cells should be same except a phase shift. This can be explained by the Bloch theorem as

$$\begin{pmatrix} A_j(n) \\ B_j(n) \end{pmatrix} = \begin{pmatrix} A_{j+1}(n) \\ B_{j+1}(n) \end{pmatrix} \exp(-iKd) \tag{7}$$

here K is a Bloch wave vector and d is the period of a unit cell. It is clear that K is limited by the first Brillouin zone via $-\pi/d \le K \le \pi/d$. Thus, we can obtain the dispersion relation of the superlattice from Eqs. (5) and (7) as

$$K = \frac{1}{d}\arccos\left[\frac{1}{2}(M_{11}(n) + M_{22}(n))\right], \tag{8}$$

where $M_{11}(n)$ and $M_{22}(n)$ are the elements of the transfer matrix for the nth cell [22].

Now, using Eqs. (6) and (8), the electron band structure and the electronic transmission coefficient be evaluated for a given superlattice structure, respectively.