Electronic band-structure engineering of GaAs/Al\(_x\)Ga\(_{1-x}\)As quantum well superlattices with substructures

Mingrong Shen\(^{a,b,*}\), Wenwu Cao\(^{a,c}\)

\(^{a}\) Materials Research Institute, The Pennsylvania State University, University Park, PA 16802, USA
\(^{b}\) Department of Physics, Suzhou University, Suzhou 215006, China
\(^{c}\) Department of Mathematics, The Pennsylvania State University, University Park, PA 16802, USA

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Abstract

We report a theoretical investigation on the band structures of electrons in both infinite and finite semiconductor quantum well/barrier superlattices with each unit cell containing alternately two types of materials. When the unit cell of a superlattice, made of GaAs and Al\(_x\)Ga\(_{1-x}\)As, is further divided into four and six sublayers of these two materials, narrower passbands and/or broad stopbands can be obtained for electrons with energy slightly larger than the potential barrier. When a finite superlattice has two different periods and each unit cell contains six sublayers of alternating GaAs and Al\(_x\)Ga\(_{1-x}\)As, very sharp passbands can be obtained for electron energy right below and above the potential barrier. The results may be used to build a high-Q electron energy filter.

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1. Introduction

Advances in the growth technology of semiconductors have made it possible to fabricate complicated semiconductor microstructures, which can be used to regulate the motion of electrons. In particular, one-dimensional semiconductor superlattices consisting of alternating ultrathin layers of different composition or different levels of doping have been obtained using molecular beam epitaxy (MBE) and metal-organic chemical vapor deposition (MOCVD). The thickness of the layers is on the scale of the de Broglie wavelength of an electron. One of the motivations to study semiconductor superlattices lies in their possible applications as new devices, for example, electron energy filter, because the electronic responses of such devices can be tailored by varying the composition and thickness of these layers [1,2]. Due to the relatively longer mean free path of the electrons compared with the spacing of the semiconductor superlattices, electrons moving in a semiconductor superlattice can experience many periods before losing their phase coherence. As a result, superlattice minibands can be formed, which superimpose onto the conduction and valence bands of the host semiconductor materials.

The electronic, transport, and optical properties of periodic and aperiodic semiconductor superlattices have been systematically studied, both experimentally and theoretically [3–9]. However, most of the reported works on periodic semiconductor superlattices were focused on layered structures consisting of only two sublayers in one unit cell. The aim of present work is to investigate theoretically the changes of the dispersion relations in infinite semiconductor superlattices and the transmission coefficient of electron waves in finite periodic superlattice structures with each unit cell containing several sublayers of the two materials. We also use finite size superlattices of multiple periodicities to regulate the mini-band-structure, analogous to our
recent study on acoustic bandgap engineering [10], but the unique quantum resonance tunneling effects of electrons bring some new and interesting physics into the superlattice problem. The theoretical study was carried out mainly within the framework of the Kronig–Penny (KP) model [11] and the use of the transfer matrix method. Although first principles calculations of superlattice structure, which use 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 [12]. On the other hand, for potential barrier thickness greater than 20 Å, the KP model is a reasonable approximation for the calculation of band structures of non-interaction electrons in infinite semiconductor superlattices [13].

In Section 2, the dispersion relations of electrons in infinite periodic semiconductor superlattices with each unit cell contains several sub-layers of two kinds of materials are derived. We use the GaAs/AlxGa1-xAs semiconductor superlattice as an example with each unit cell containing alternatingly two, four and six sublayers, respectively, of GaAs and AlxGa1-xAs of different thickness. Transmission coefficients were studied for cases with the electron energy both below and above the barrier height. In Section 3, we introduce an extension to the transfer matrix technique, which enables us to calculate the band structures of finite size superlattice without using the Bloch theorem. The transmission coefficient was calculated as a function of electron energy. In Section 4, a special structure of superlattice with two sub-periodic-structures is studied, which can be used as high-Q electron energy filter with extremely narrow passbands. Section 5 contains the summary and conclusions.

2. Dispersion relations for infinite semiconductor superlattice

First, we consider an infinite semiconductor superlattice made of two different materials \( X \) and \( Y \). Each unit cell contains \( M \) layers of \( X \) and \( Y \) with different thickness, and we use \((X_1 Y_1 X_2 Y_2 \ldots X_M Y_M)_{n} \) to represent the \( n \)th unit cell. The thickness of these layers are \( d_{X1}, d_{Y1}, d_{X2}, d_{Y2}, \ldots, d_{XM}, d_{YM} \), respectively. These layers form quantum wells/barriers for the electron waves as depicted in Fig. 1.

When an electron with energy above the potential barrier \( V_0 \) is incident normal to the layered structure, the wave function at the \( j \)th layer of the \( n \)th cell can be written in the following form by solving the Schrodinger’s equation:

\[
\psi_{nj} = a_{nj} e^{-ik_{nj}z} + b_{nj} e^{ik_{nj}z}
\]  

where \( n \) is the unit cell number, and \( j \) is the layer number within the \( n \)th cell. The first term on the right hand side of Eq. (1) represents the forward wave and the second term represents the reflecting wave, and \( k_j \) is the wave vector for electron propagating in the \( j \)th material given by:

\[
\frac{\hbar k_j^2}{2m_{X}} = \varepsilon \quad \text{(in material \( X \))}
\]

\[
\frac{\hbar k_j^2}{2m_{Y}} = \varepsilon - V_0 \quad \text{(in material \( Y \))}
\]

where \( \varepsilon \) is the energy of the electron measured from the potential level of material \( A \) (bottom of the well), and \( m_{X} \) and \( m_{Y} \) are the electron effective masses in \( X \) and \( Y \), respectively. Note that \( k_y \) becomes pure imaginary when \( \varepsilon < V_0 \). This case represents the situation inside the energy barrier and the wave function Eq. (1) becomes exponential functions without wave characteristics. Interestingly, resonance tunneling will occur for such situation as discussed below. For the superlattice of GaAs/AlxGa1-xAs, the relation between the effective masses and the Al content \( x \) is [13]:

\[
m_{X} = 0.067 m_{0}, \quad m_{Y} = (0.067 + 0.083x) m_{0}
\]

where \( m_{0} \) is the bare electron mass. By applying the appropriate boundary conditions at the interface between materials \( X \) and \( Y \) we have [14,15]:

\[
\psi_{X}|_{\text{boundary}} = \psi_{Y}|_{\text{boundary}}.
\]
\[
\frac{1}{m_X} \frac{\partial \psi_X}{\partial z} \bigg|_{\text{boundary}} = \frac{1}{m_Y} \frac{\partial \psi_Y}{\partial z} \bigg|_{\text{boundary}}.
\]

The continuity equations Eq. (5a,b) leads to the following relations among the coefficients \(a_{n,j}, b_{n,j}\) and \(a_{n+1,j}, b_{n+1,j}\) for two adjacent cells

\[
\begin{pmatrix}
a_{n,j} \\
b_{n,j}
\end{pmatrix} =
\begin{pmatrix}
A & B \\
C & D
\end{pmatrix}
\begin{pmatrix}
a_{n+1,j} \\
b_{n+1,j}
\end{pmatrix}
\]  

where the 2 \( \times \) 2 transfer matrix is given by:

\[
\begin{pmatrix}
A & B \\
C & D
\end{pmatrix} = \prod_{j=1}^{M} \begin{pmatrix}
A_j & B_j \\
C_j & D_j
\end{pmatrix}
\]  

with

\[
A_j = \frac{w_j + w_{j+1}}{2w_j} e^{ikjd}z_j
\]

\[
B_j = \frac{w_j - w_{j+1}}{2w_j} e^{ikjd}z_j
\]

In Eq. (7) \(C_j\) and \(D_j\) are the complex conjugates of \(B_j\) and \(A_j\), respectively, \(z_j\) is the coordinate of the interface between the \(j\)th and \((j+1)\)th layers, and \(w_j = k_j/m_j\), which is imaginary if the electron energy is less than the barrier height.

According to the Bloch theorem, for an infinite superlattice, the coefficients \(a_{n,j}\) and \(b_{n,j}\) for the same material in different unit cells must be the same except a phase shift and can be expressed as:

\[
\begin{pmatrix}
a_{n,j} \\
b_{n,j}
\end{pmatrix} = \begin{pmatrix}
a_{n+1,j} \\
b_{n+1,j}
\end{pmatrix} e^{-ikd}
\]  

where \(k\) is the Bloch wave vector defined over the first Brillouin zone \((-\pi/d < k \leq \pi/d)\), and \(d\) is the period of a unit cell.

The dispersion relation can be obtained from equation Eqs. (6) and (8),

\[
k = \frac{1}{d} \arccos \left[ \frac{1}{2} (A + D) \right]
\]

where

\[
A + D = \prod_{h=1}^{M} \cos(k_d d_h)
\]

\[
- \sum_{h=1}^{M-1} \prod_{h=1}^{M} \left[ \left( \frac{w_h + w_j}{w_j} \right) \sin(k_d d_h) \sin(k_d d_j) \right]
\]

\[
\times \prod_{l \neq h, j = 1}^{M} \cos(k_d d_j)
\]

\[
 \sum_{h=1}^{M-3} \sum_{j=1+2}^{M-1} \sum_{k=h+1}^{M-1} \left[ \left( \frac{w_h w_j}{w_j} \right) \sin(k_d d_h) \sin(k_d d_j) \right]
\]

\[
\times \prod_{n \neq h, j, k, l, m, n, p, q, r, s = 1}^{M} \cos(k_d d_j)
\]

The calculated dispersion relations for electrons of (energy larger than \(V_0\)) propagating through infinite superlattice with each cell containing two, four or six layers of alternating GaAs and Al\(_{0.3}\)Ga\(_{0.7}\)As are shown in Fig. 2. In each case, the volume ratio of GaAs and Al\(_{0.3}\)Ga\(_{0.7}\)As was kept constant so that the cell period is kept at \(d = 18\) nm. Fig. 2(a) is a typical dispersion relation for an infinite semiconductor superlattice formed by two sublayer unit cells. The piecewise
dispersion curves represent the passbands and the gaps are the stopbands. If the unit cell is subdivided into four sublayers of alternating GaAs and Al\textsubscript{0.3}Ga\textsubscript{0.7}As, flatter passbands and wider stopbands are formed. This trend is confirmed by further subdividing the unit cell into six layers of alternating GaAs and Al\textsubscript{0.3}Ga\textsubscript{0.7}As as shown in Fig. 2(c). It is also noted that the first passband shifts down to lower energy when the unit cell is divided into more sublayers. Fig. 3 corresponds to the case when the electron energy is lower than the barrier height $V_0$. All parameters are the same as given in the caption of Fig. 2.

The Bloch theorem is only valid for an infinite system for which periodic condition holds. This does not reflect real experimental situations since the measured structures are always finite in size. Band structures are incomplete for a finite system although the shape could be similar to that of the infinite system, therefore, it is more meaningful to study the frequency spectrum of the transmission coefficient for finite systems.

3. Energy spectrum of the transmission coefficient for finite size superlattices

Considering a finite system of N cells, we can derive the following relation, according to the recurrence relation Eq. (6):

$$
\begin{pmatrix}
a_{N+1,1} \\
b_{N+1,1}
\end{pmatrix} = [T] \begin{pmatrix}
a_{N,1} \\
b_{N,1}
\end{pmatrix}
$$

(12)

where the T matrix in Eq. (12) is a second rank tensor given by:

$$
[T] = \prod_{n=1}^{N} \begin{pmatrix}
A_n & B_n \\
C_n & D_n
\end{pmatrix}.
$$

(13)

Assuming the electron is incident from the left (GaAs), only a transmitted wave exists in the right hand side of the superlattice (also GaAs), that is $b_{N+1,1} = 0$.

Now let us define a transmission function $H(\varepsilon)$, analogous to acoustic waves in one dimensional finite periodic structures [16],

$$
H(\varepsilon) = \frac{a_{N+1,1}}{d_{1,1}} e^{-\imath k_x N d} = \frac{1}{T_{11}} e^{-\imath k_x N d},
$$

(14)

which describes both the amplitude and phase relationships between the incident electron wave at $z = 0$ and the transmitted wave at $z = N d$. The transmission coefficient is given by:

$$
t = H(\varepsilon) \cdot H^*(\varepsilon)
$$

(15)

Fig. 3. The dispersion curves for the case shown in Fig. 2 with the electron energy blow the barrier height $V_0$. All parameters are the same as given in the caption of Fig. 2.

Fig. 4. Calculated energy spectrum of the transmission coefficient for finite size superlattices ($N = 20$). (a) Two sublayers, (b) four sublayers and (c) six sublayers. The corresponding parameters used for the calculations are the same as those given in Fig. 2.
Fig. 4 shows the calculated energy spectra of the transmission coefficient for one unit cell containing two, four and six layers of alternating GaAs and Al\textsubscript{0.3}Ga\textsubscript{0.7}As. The total number of cells is 20 for this calculated structure. Other parameters used are the same as for the case given in Fig. 2. The band ranges are consistent with that of Figs. 2 and 3, therefore, the definition of the transmission coefficient is appropriate. We found that sharp passbands and wider stopbands could be obtained when the unit cell was divided into more sublayers. Gipps-type oscillations were seen in the passbands, which come from the finite nature of the system. Complete transmission, i.e. \( t = 1 \), can be achieved at isolated energies due to the resonance nature of the electron wave. The stopbands corresponds to total reflection, i.e. \( t = 0 \). For a finite system, such condition cannot be achieved, but the value of \( t \) can become negligibly small as \( N \) increases. Resonance tunneling can occur for multiple periodic barriers and the passbands are much narrower compared with the passbands above the energy barrier.

The bandgaps can also be adjusted through changing the volume ratio of GaAs and Al\textsubscript{1-x}Ga\textsubscript{x}As. In Fig. 5, we showed the effects where the total barrier thickness is increased. The ratios of total thickness of the barriers to that of the wells in one unit cell are, respectively, 0.5 [Fig. 5(a)], 1.0 [Fig. 5(b)], and 2.0 [Fig. 5(c)]. It can be seen that narrow passbands can be obtained when the ratio increases, and the passbands also shift to higher energies both below and above the barrier height \( V_0 \).

Because the mean free path of the electrons is finite, numerical calculations for a finite number of periods are more meaningful. On the other hand, our study indicated that a finite number of cells could already support a well-defined band structures.

4. A finite superlattice with two periodic substructures

We consider a finite superlattice containing two substructures of different periods. The main objective here is to use the idea of band-gap engineering to fabricate quantum well/barrier structures that have very narrower passbands for filter applications. Each substructure of the superlattice can produce its own band structure as discussed in previous section. If the passbands of the two substructures are not overlapped in certain energy range, the probability for the electron to pass through the whole structure will be low, which creates a broader stopband; if they are partially overlapped, only the overlapped part of energy band allow electrons to pass, thus, a narrow band electron energy filter is obtained.

The condition to realize the above idea is that both superlattices should have relatively broad stopbands to begin with. The results in Section 3 shows that we can use the superlattice with unit cell containing six sublayers of GaAs and Al\textsubscript{1-x}Ga\textsubscript{x}As to obtain broad stopbands in the electron energy range above \( V_0 \) (=240 meV in our calculation). Fig. 6 shows the calculated energy spectrum of the transmission coefficient for the superlattices containing two different sub-superlattices. Each substructure has 20 unit cells so that the whole structure contains 40 cells in total. It is interesting to see that two very narrow passbands centered at about 163 and 437 meV, respectively, were indeed obtained in the energy ranges slightly below and slightly above \( V_0 \). As the electron energy increases, the effects of the barriers become weaker. When the electron energy is more than two times higher than the barrier height, \( \varepsilon > 2V_0 \), the superlattice idea cannot be used to design energy filter since the stop bands are very narrow to begin with as shown in Fig. 4 for the electron energy greater than 500 meV.

![Fig. 5. Change of energy spectrum of the transmission coefficient for a finite superlattice \((N = 20)\) with six sublayers in one unit cell. The volume ratios of \( \text{Al}_{0.3}\text{Ga}_{0.7}\text{As} \) are: (a) 1/3; (b) 1/2 and (c) 2/3, respectively. The corresponding thickness of each sublayer is given by: (a) \( d_{x1} = 2 \) nm, \( d_{y1} = 2 \) nm, \( d_{x2} = 4 \) nm, \( d_{y2} = 2 \) nm, \( d_{x3} = 6 \) nm, and \( d_{y3} = 2 \) nm. (b) \( d_{x1} = 2 \) nm, \( d_{y1} = 3 \) nm, \( d_{x2} = 3 \) nm, \( d_{y2} = 5 \) nm, \( d_{x3} = 4 \) nm, and \( d_{y3} = 3 \) nm. (c) \( d_{x1} = 2 \) nm, \( d_{y1} = 2 \) nm, \( d_{x2} = 2 \) nm, \( d_{y2} = 4 \) nm, \( d_{x3} = 2 \) nm, and \( d_{y3} = 6 \) nm.](image1)

![Fig. 6. Calculated energy spectrum of the transmission coefficient for a superlattice structure containing two sub-superlattices. The thickness values in one of the superlattices are: \( d_{x1} = 2 \) nm, \( d_{y1} = 2 \) nm, and \( d_{y3} = 2 \) nm. And in the other type of cells are: \( d_{x'1} = 2 \) nm, \( d_{y'1} = 2 \) nm, \( d_{y'2} = 4 \) nm, \( d_{x'2} = 2 \) nm, and \( d_{y'3} = 6 \) nm.](image2)
5. Summary and conclusions

Electronic bandgaps produced by semiconductor superlattices stem from the wave characteristics of electrons. In this paper, we have investigated two types of superlattices and their associated energy band structures. The first is a quantum well/barrier superlattice with each unit cell containing several sublayers of two materials in alternate positions. Numerical calculations of the dispersion relation for an infinite superlattice and transmission coefficient for a finite GaAs/Al$_x$Ga$_{1-x}$As superlattice showed that when the electron energy is comparable to potential barrier height, narrow passbands and/or broad stopbands can be obtained when the unit cell is divided into four or more sublayers. The bandgap can also be adjusted through changing the total volume ratio of Al$_x$Ga$_{1-x}$As and GaAs in one unit cell. When the ratio of Al$_x$Ga$_{1-x}$As to GaAs increases, narrower passbands can be obtained and each passband also moves to higher energy. Another design of quantum well/barrier structure is to combine two sub-superlattices of different periods with each unit cell containing six sublayers of alternating GaAs and Al$_x$Ga$_{1-x}$As. Two very narrow passbands were obtained in the vicinity of the barrier height $V_0$. Our results showed that it is possible to produce high-Q electron energy filters with narrow peaks of transmission coefficient using quantum well/barrier superlattices with unit cells containing substructures. Experimentally, photoreflectance spectroscopy is an accurate method for the characterization of multiple-quantum-well structures [17]. It is would be interesting to verify our theoretical results using this technique.

References