ELECTRON ENERGY STATES AND MINIBAND PARAMETERS IN A CLASS OF NON-UNIFORM QUANTUM WELL AND SUPERLATTICE STRUCTURES

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A simple method to compute the carrier energy states, miniband parameters and dispersion characteristics for single and multiple quantum well and superlattice structures is presented. The method utilizes the continuity of the envelope function across the heterojunctions according to the boundary conditions that both the wavefunction ψ and the particle current density ψ'/m^* be continuous at each interface. The nonuniform potential distribution encountered in doped or compositionally graded materials is approximated by piecewise constant potential functions. In addition to being conceptually simple, the method is readily adopted to fairly complex structures where other more sophisticated methods such as LCAO, reduced Hamiltonian and tight binding theories may become unfeasible or unmanageable. It is shown that for an arbitrary stepped potential variation, the eigenvalues (or the energy states) of quantum wells or a finite number of coupled quantum wells can be found by utilizing a transverse resonance method which is readily implemented on a digital computer for the computation of these eigenvalues. For the case of periodic superlattices, the miniband parameters and the dispersion characteristics are computed from a suitably defined transmission matrix associated with a unit cell of the superlattice which may itself consist of multiole layers. Typical results for the computed parameters for several wells and simple, biperiodic, binary and polytype superlattices consisting of various $Al_xGa_{1-x}As$ and $In_xGa_{1-x}As$ alloys are presented.

I. INTRODUCTION

A considerable amount of work has been done in recent years on the evaluation of the electronic properties of various compositional and doped quantum well and superlattice structures.[1-10] One of the most successful methods used in deriving the eigenvalue equations for quantum wells and dispersion equations for periodic structures has been the use of plane wave type solutions with assumed[1-3] or derived[6,7,11,12] boundary conditions or connection rules. Even though more accurate methods such as LCAO[5], reduced Hamiltonian[9] and other microscopic theories[8] are available particularily for thin structures, the wave equation approach with appropriate boundary conditions[11,12] is conceptually simple and can be readily applied to the multilayered wells and simple and polytype[13] superlattice problems. In this paper a unified systematic approach that utilizes a transverse resonance condition for quantum wells and a transmission matrix method for periodic structures is presented.

II. THEORY

The eigenvalues of the quantum wells and multiple coupled quantum wells and the miniband parameters of periodic quantum well structures are found by

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solving the one-dimensional Schrodinger wave equation with the potential variation specified by the conduction and valence band discontinuities[14]. It is assumed that each layer contains a sufficient number of atomic sublayers such that the effect of atomic potentials in each region can be assumed to be at least partly included in the effective mass. Each layer acts like a crystal modified at most by a slowly varying potential and the effective mass wave function is a modulated Bloch wave with an envelope governed by the Schrodinger equation. In addition, the layers are assumed to be sufficiently thin with low doping levels such that they are modelled by wells and barriers of uniform thickness even in the presence of an applied bias voltage. The interface connection rules for the effective mass wave function at the abrupt heterojunctions correspond to the continuity of the slowly varying envelope function introduced by Bastard[6] and subsquently reinforced by White et. al.[11] Alternately, the connection rules derived by Kroemer and Zhu[12] may be utilized which will obviously lead to slightly different results depending upon the discontinuity in effective mass across the interface. That is, the wave function in the jth region is a solution of

$$\frac{d^2\psi_j}{dz^2} + \frac{2m_j^*}{\hbar^2}(E-V_j)\psi_j = 0 \qquad (1)$$

with $\frac{1}{m_j^*}\frac{d\psi_j}{dz}$ and ψ_j being continuous across the heterojunction if the continuity of envelope function as derived by Bastard[6,7] for type I superlattices (e.g., GaAs-$A\ell_xGa_{1-x}As$)is to be utilized. It should be mentioned that both boundary conditions conform to the continuity of the probability current density. In addition, for the case of type II (InAs-GaSb type) superlattices where the periodic part of the host material Bloch function cannot be neglected, the corresponding connection rules for the envelope function[7] can be utilized.

The solution of the above equations for simple cases of potential wells and superlattices are well known. For more complex stepped or graded potential variation due to compositional changes in the structure, it is convenient to solve for the eigenvalues of quantum wells and dispersion characteristics of periodic structures by utilizing known results for analogous systems in layered media, cascaded guided wave structures and other engineering problems. It is to be noted that we do not necessarily have to utilize this analogy in that all the results can be obtained by constructing the solution of the wave equation subject to the given boundary conditions.

In the notation of linear system theory the state vector $x]$ characterizing the one dimensional system is a solution of:

$$\frac{d}{dz}\,x] = [A]x] \qquad (2)$$

where $x] \triangleq \begin{matrix} x_1 \\ x_2 \end{matrix}] = \begin{matrix} \psi \\ \frac{1}{jm^*}\frac{d\psi}{dz} \end{matrix}]$ and then the characteristic matrix is given by

$$[A] = \begin{bmatrix} 0 & -jm^* \\ -j\frac{2(E-V)}{\hbar^2} & 0 \end{bmatrix}.$$ The state variables x_1 and x_2 are continuous at the heterojunctions between individual layers.

The solution of the wave equation in each layer can now be expressed in terms of a propagation constant and a characteristic impedance which are given by

$$\gamma = \sqrt{\frac{2m^*(V-E)}{\hbar^2}} \qquad (3)$$

and

$$Z_o = \sqrt{\frac{m^*\hbar^2}{2(E-V)}} \qquad (4)$$

The characteristic impedance parameter represents the ratio $[\psi/\frac{1}{jm^*}\frac{d\psi}{dz}]$ associated with an electron wave traveling in the positive z direction. It should be noted that in the regions where E<V, γ is real and Z_o imaginary and the solution represents evanescent modes. Each layer of width ℓ is completely characterized in terms of γ and Z_o given above and the solution of complex boundary value (multiple interface) problems can be facilitated by recalling some of the transmission and translational properties of $x]$. The transmission matrix for the two variables is given by

$$\begin{matrix} \psi \\ \frac{1}{jm^*}\frac{d\psi}{dz} \end{matrix}\Bigg]_{\text{at } z=\ell} = \begin{bmatrix} \cosh\gamma\ell & Z_o\sinh\gamma\ell \\ \frac{\sinh\gamma\ell}{Z_o} & \cosh\gamma\ell \end{bmatrix} \times$$

$$\left.\frac{\psi}{\frac{1}{jm^*}\frac{d\psi}{dz}}\right]_{\text{at } z=0} \qquad (5)$$

The translational property is characterized in terms of the impedance $(\psi/\frac{1}{jm^*}\frac{d\psi}{dz})$ seen at a distance ℓ from a discontinuity. For example, if $Z_{\ell_1} \triangleq [\psi/\frac{1}{jm^*}\frac{d\psi}{dz}]$ is specified at a given plane ($z=\ell_1$) then the impedance at a distance ℓ from that plane is given by

$$\left.\frac{\psi}{\frac{1}{jm^*}\frac{d\psi}{dz}}\right|_{\text{at } z=\ell_1-\ell} = Z_o \frac{Z_{\ell_1}+Z_o\tanh\gamma\ell}{Z_o + Z_{\ell_1}\tanh\gamma\ell} \qquad (6)$$

III. QUANTUM WELL STRUCTURES

For the case of isolated or coupled quantum well structures, represented by a finite number of stepped potential regions, the eigenvalues are found by utilizing the transverse resonance condition. That is, the net $(\psi/\frac{1}{jm^*}\frac{d\psi}{dz})$ or total impedance is either zero or infinity at every plane along the structure. In order to illustrate the procedure, we consider the case of the symmetrical stepped potential strucutre shown in Table I, case (d). The total impedance at the axis of symmetry is readily found by utilizing the translational property of impedance as given by eqn. (6) and is found to be

$$Z\Big|_{\substack{\text{at the}\\ \text{axis}\\ \text{of symmetry}}} = \frac{Z_1}{2}\left\{\frac{Z_2\frac{Z_3+Z_2\tanh\gamma_2\ell_2}{Z_2+Z_3\tanh\gamma_2\ell_2} + Z_1\tanh\gamma_1\frac{\ell_1}{2}}{Z_1+Z_2\frac{Z_3+Z_2\tanh\gamma_2\ell_2}{Z_2+Z_3\tanh\gamma_2\ell_2}\tanh\gamma_1\frac{\ell_1}{2}}\right\}.$$

Setting this impedance equal to 0 or ∞ leads to eigenvalues asociated with odd- and even-eigenfunctions respectively. These eigenvalue equations together with other typical cases are given in Table I.

IV. PERIODIC STRUCTURES

The dispersion equation for the periodic structures or the superlattices is readily derived by utilizing the tranmission matrix as given by Eqn. (5). The overall transmission matrix of the unit cell of a periodic structure where the unit cell itself consists of N layers, is given by,

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix} = \prod_{j=1}^{N} \begin{bmatrix} \cosh\gamma_j\ell_j & Z_j\sinh\gamma_j\ell_j \\ \frac{1}{Z_j}\sinh\gamma_j\ell_j & \cosh\gamma_j\ell_j \end{bmatrix} \qquad (8)$$

Then the dispersion equations for the periodic structure are readily found in terms of the elements of the ABCD matrix and is given by

$$\frac{A+D}{2} = \cos k\,d \qquad (9)$$

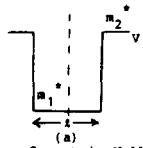
where d is the total length of each unit cell ($= \sum_{j=1}^{N} \ell_j$) and k is the wave number. The derivation of the dispersion equation then simply ammounts to multiplying the transmission matrices to find overall transmission parameters A and D and is given in Table II for the cases of a simple and an ABC polytype superlattice.

V. RESULTS AND DISCUSSION

The eigenvalue equations for quantum well structures are of the form $F_1(E,p_1,p_2,..p_n)=0$ and the dispersion equations for periodic structures are of the form $F_2(E,p_1,p_2,..p_n)-\cos kd=0$. In both cases $p_1..p_n$ are known variables such as effective mass and potential associated with the individual layers. The effect of nonparabolicity of the conduction and valence band of each layer can be included in the effective mass[14]. A convenient method to solve these equations is the use of standard multiple variable optimization programs[15]. Here we define a utility function $|F_1|^2$ for quantum well problems and $|F_2-\cos kd|^2$ for superlattice dispersion problems and seek the minima (zeros) of the utility function with energy as a variable. The eigenvalues for some quantum well structures and the miniband parameters such as the dispersion diagrams are shown in Figs. (1)-(5) for some typical cases of wells and superlattices consisting of various $Al_xGa_{1-x}As$ and $In_xGa_{1-x}As$ alloys.

A unique, and useful feature of the optimization procedure chosen to compute the characteristic solutions for quantum well structures is its amenability to design synthesis of such structures. We can solve for a set of parameters p_i, p_{i+1}, ..., p_{i+j} such that the remainder parameters p_1, p_2, ..., p_{i-1}; p_{i+j+1}, p_n have desired specified values for a system of n variables. A trivial

Table I: Schematics and eigenvalue equations for various stepped-potential structures.

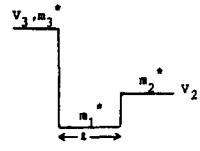


(a)
Symmetric Well

$$\tan\sqrt{\frac{2m_1^* E}{\hbar^2}}\frac{t}{2} = -\sqrt{\frac{m_2^* E}{m_1^*(V-E)}} \quad \text{(odd)}$$

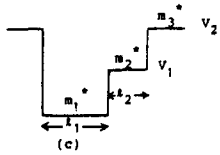
or

$$\tan\sqrt{\frac{2m_1^* E}{\hbar^2}}\frac{t}{2} = -\sqrt{\frac{m_1^*(V-E)}{m_2^* E}} \quad \text{(even)}$$



(b)
Non-Symmetrical Well.

$$\tan\sqrt{\frac{2m_1^* E}{\hbar^2}}\,t = -\frac{\sqrt{\frac{m_2^* E}{m_1^*(V_2-E)}}+\sqrt{\frac{m_3^* E}{m_1^*(V_3-E)}}}{1+\sqrt{\frac{m_2^* m_3^*}{m_1^{*2}}}\frac{E^2}{(V_2-E)(V_3-E)}}$$

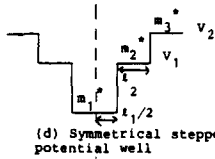


(c)
Asymmetric stepped potential well

$$\tan\sqrt{\frac{2m_1^* E}{\hbar^2}}\,t = -\frac{K_A + K_B}{1 + K_A K_B}$$

where $K_A = \sqrt{\frac{m_3^* E}{m_1^*(V_3-E)}}$

$$K_B = \sqrt{\frac{m_2^* E}{m_1^*(V_2-E)}}\left\{\frac{\sqrt{\frac{m_3^*}{m_1^*}\frac{(V_2-E)}{(V_3-E)}}+\tanh\sqrt{\frac{2m_2^*}{\hbar^2}(E-V_2)}\,t_2}{1+\sqrt{\frac{m_3^*(V_2-E)}{m_2^*(V_3-E)}}\tanh\sqrt{\frac{2m_2^*(E-V_2)}{\hbar^2}}\,t_2}\right\}$$

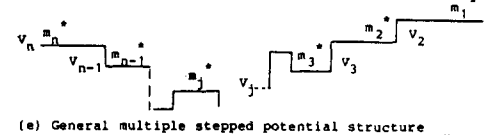


(d) Symmetrical stepped potential well

$$\tan\sqrt{\frac{2m_1^* E}{\hbar^2}}\frac{t_1}{2} = -\sqrt{\frac{m_2^*}{m_1^*}\frac{E}{(V_2-E)}}\,K; \quad \text{(odd)}$$

$$\tan\sqrt{\frac{2m_1^* E}{\hbar^2}}\frac{t_1}{2} = -\sqrt{\frac{m_1^*(V_2-E)}{m_2^* E}}\frac{1}{K} \quad \text{(even)}$$

where, $K = \dfrac{\sqrt{\frac{m_3^*}{m_2^*}\frac{(V_2-E)}{(V_3-E)}}+\tanh\sqrt{\frac{2m_2^*}{\hbar^2}(E-V_2)}\,t_2}{1+\sqrt{\frac{m_3^*(V_2-E)}{m_2^*(V_3-E)}}\tanh\sqrt{\frac{2m_2^*(E-V_2)}{\hbar^2}}\,t_{2(E<V_1)}}$ (odd)



(e) General multiple stepped potential structure

$$z_j = \sqrt{\frac{m_j^* \hbar^2}{2(E-V_j)}},$$

$$\gamma_j = \sqrt{\frac{2m_j^*(V_j-E)}{\hbar^2}}; \quad j=1,2\ldots n$$

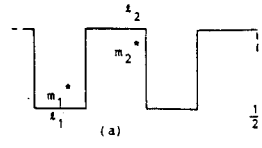
$$z_1' = z_1,$$

$$z_2' = z_2\,\frac{z_1' + z_2\tanh\gamma_2 t_2}{z_2 + z_1'\tanh\gamma_2 t_2};$$

$$z_{j+1}' = z_j\,\frac{z_{j-1}' + z_j\tanh\gamma_j t_j}{z_j + z_{j-1}'\tanh\gamma_j t_j};$$

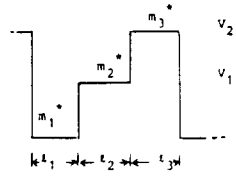
$$z_n' + z_n = 0 \text{ (eigenvalue equation)}$$

Table II Schematics and Dispersion Relation for Two Superlattice Structures



Simple AB type SL

$$\frac{1}{2}\sin\beta_1 t_1 \sinh\gamma_2 t_2 \left[\frac{\gamma_2}{\beta_1}\frac{m_1^*}{m_2^*} - \frac{\beta_1}{\gamma_2}\frac{m_2^*}{m_1^*}\right] + \cosh\gamma_2 t_2 \cos\beta_1 t_1 = \cos k(t_1+t_2);\ 0<E<V$$



ABC polytype SL*

$$\cos\beta_1 t_1\{2\cosh\gamma_2 t_2 \cosh\gamma_3 t_3 + \sinh\gamma_2 t_2 \sinh\gamma_3 t_3\{\frac{z_2}{z_3}+\frac{z_3}{z_2}\}\}$$

$$+ j\sin\beta_1 t_1\{\sinh\gamma_2 t_2 \cosh\gamma_3 t_3\{\frac{z_1}{z_2}+\frac{z_2}{z_1}\} + \sinh\gamma_3 t_3 \cosh\gamma_2 t_2\{\frac{z_1}{z_3}+\frac{z_3}{z_1}\}\} = \cos k(t_1+t_2+t_3);\ 0<E<V_1$$

* The dispersion equations for these cases and for ABCD polytype SL are given in Reference 7.

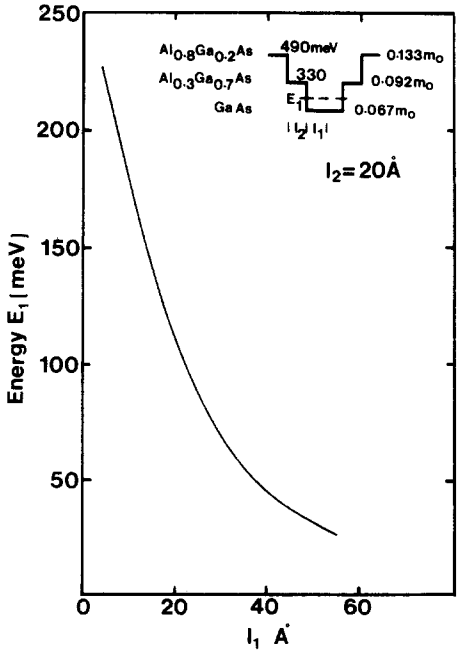


Figure 1 Variation of electron subband (n=1) energy in a symmetrical stepped-potential GaAs-$Al_xGa_{1-x}As$ quantum well.

example would be: given a simple GaAs - $Al_{0.3}Ga_{0.7}As$ superlattice, to calculate the well and barrier lengths such that the superlattice has a desired effective energy band gap and band width. This problem is easily solved by simply looking at the plots of miniband energy parameters as a function of the two lengths and the results are found to be the same.

IV. CONCLUSIONS

A unified approach to analyze and compute the eigenvalues of a class of nonuniform general stepped potential quantum well strucutes and miniband parameters of superlattices consisting of such coupled quantum wells has been formulated. A transverse resonance method for the derivation of the quantum well eigenvalue equations and a transmission matrix approach for the derivation of the dispersion equation for the periodic structures has been used to compute the characteristic parameters of some typical structures. The methodology presented is applicable to fairly complex structures with multiple layers where other more accurate computational methods become unfeasable. In addition to help

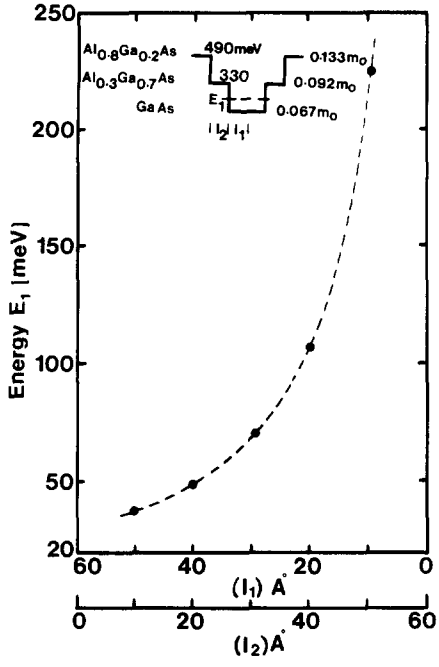


Figure 2 Variation of electron subband (n=1) energy with step dimension in a symmetrical stepped potential GaAs-$Al_xGa_{1-x}As$ quantum well.

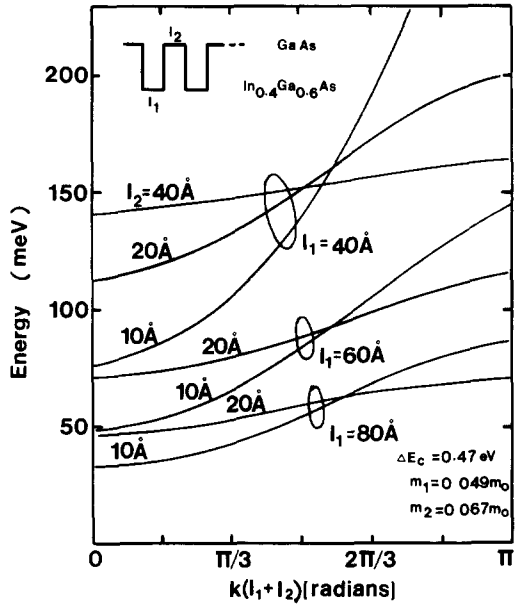


Figure 4 E-k diagrams for a $In_{0.4}Ga_{0.6}As$ - GaAs strained layer superlattice.

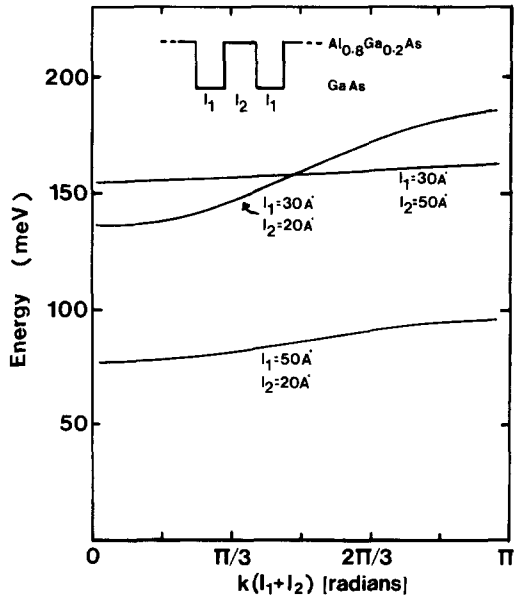


Figure 3 E-k diagram for a $Al_{0.8}Ga_{0.2}As$ - GaAs superlattice.

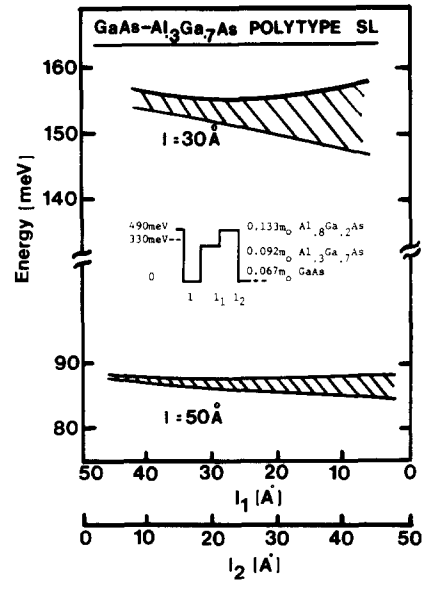


Figure 5 Width of the first miniband as a function of barier thickness l_2 in a GaAs - $Al_{0.3}Ga_{0.7}As$ - $Al_{0.8}Ga_{0.2}As$ polytype superlattice.

predicting the electronic properties of various quantum well and superlattice structures, the analytical and numerical techniques described are adaptable to a design synthesis procedure for such structures via parameter optimization or other analytical techniques that have been used for analogous systems[16]. Even though the analysis and results presented in the paper are directly applicable to type I superlattices, the same procedure can be applied to the case of type II superlattices. For the latter case the state variables are redefined and the expressions for Z_j are modified such that the corresponding boundary conditions as derived by Bastard[6,7] are satisfied. That is, all of the eigenvalue and dispersion equations derived in the paper also characterize type II quantum wells and superlattices provided the expressions for Z_j are modified accordingly.

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