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Validity of the connection-matrix approach to GaAs-$Al_xGa_{1-x}As$ quantum wells

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The abruptness of the semiconductor heterojunction has been dealt with by many past researchers by incorporating the single-band effective-mass equation with a connection matrix at the interface. This connection-matrix method has been used to predict the eigenenergies of the GaAs-$Al_xGa_{1-x}As$ quantum wells. In this paper, the validity of this approach to quantum wells is examined by varying the location of the interface within a lattice constant to reveal the eigenenergy dependence on the location. The eigenenergy should be independent of the interface location if the single-band effective-mass equation combined with the connection matrix is a consistent theoretical entity. However, as the interface is displaced from $-a$ to a (where a is the lattice constant) relative to the location where the numerical values of the connection matrices are usually given in the literature, the first and the second eigenenergies of the GaAs-$Al_{0.3}Ga_{0.7}As$ quantum wells can deviate by about 6 and 20 meV, respectively. Therefore, it is concluded that the connection-matrix approach to quantum wells is not sufficiently consistent. However, the eigenenergy deviations become less signficant for the quantum well with lower barrier energy and wider well width.

I. INTRODUCTION

The effective-mass equation is valid for a slowly varying potential.[1] The abrupt change of the constituents in a semiconductor heterojunction introduces a challenging modification to the effective-mass equation. The connection matrix which connects the envelope functions and their first derivatives at the heterojunction has been devised to deal with this difficulty[2-7] and has also been applied to the computation of the eigenenergies of quantum wells and superlattices.[8,9]

The connection-matrices method is developed to combine with the effective-mass equation in order to improve the results predicted by using the effective-mass approximation, with the continuity assumption conventionally made on the envelope function and the probability flux based on the envelope function at the heterojunction.[10] The methods used for the computation of the connection matrix employ either the tight-binding model[2,4,5] or the pseudopotential model.[3,5,7]

By the tight-binding model, Ando, Wakahara, and Akera deduced an effective-mass-dependent connection matrix at the GaAs-$Al_xGa_{1-x}As$ interface.[5] By the pseudopotential method, Cuypers and van Haeringen introduced an energy-dependent connection matrix.[7] In this paper both the effective-mass-dependent and the energy-dependent connection matrices will be explored.

In a rectangular quantum well, there are two heterojunctions, and the locations of the interfaces where the connection matrices are given are arbitrary to within a lattice constant because the interfaces are artificially drawn. With this arbitrariness in mind, it is expected that the eigenenergies predicted by the single-band effective-mass equation incorporated with the connection matrix should be independent of the interface location. The purpose of this paper is to perform these eigenenergy calculations of the GaAs-$Al_xGa_{1-x}As$ quantum wells to examine the validity of this theoretical approach.

II. THE EXAMINATION METHODS

The connection matrix utilized to deal with the semiconductor heterojunction connects the envelope function and its first derivative at the interface[5,6,7]

$$\begin{bmatrix} \psi_B(z_0) \\ \nabla\psi_B(z_0) \end{bmatrix} = \mathbf{T}(z=z_0) \begin{bmatrix} \psi_A(z_0) \\ \nabla\psi_A(z_0) \end{bmatrix} , \tag{1}$$

with

$$\mathbf{T}(z=z_0) = \begin{bmatrix} t_{11} & t_{12} \\ t_{21} & t_{22} \end{bmatrix} , \tag{2}$$

where z_0 is the location of the interface. Material A is the first-grown material and is drawn on the left-hand side ($z<z_0$) as shown in Fig. 1. Material B is drawn on the right-hand side ($z>z_0$). Both materials are assumed to have single-band extrema, and the band extrema are close in energy.[1,5,11] ψ_A and ψ_B are the envelope functions in materials A and B, respectively. $\nabla = a\,d/dz$, with a being the lattice constant. $\mathbf{T}(z=z_0)$ is the 2×2 connection matrix with the dimensionless matrix elements of t_{11}, t_{12}, and t_{21}, and t_{22}.

One way to calculate the connection matrix is by the linear chain model of the constituent atoms, each kind of which contributes either s orbitals or p orbitals.[2,4,5] The transfer integrals are only considered between the nearest neighbors.[12] Another way is by the empirical pseudopotential method.[7] The connection conditions for the envelope functions at the interface are obtained by matching the wave functions on both sides of the interface in order for the overall wave function to become smooth at the heterojunction.

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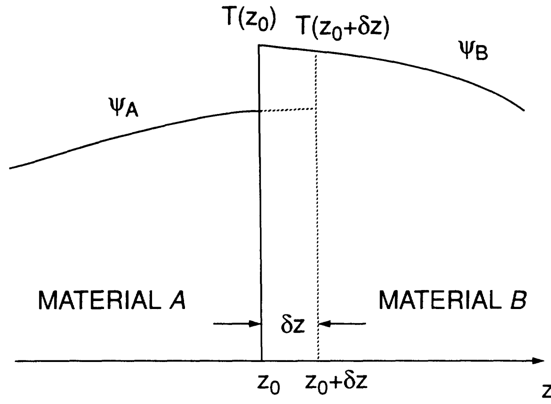

FIG. 1. A semiconductor heterojunction. A semiconductor heterojunction is sketched. The first-grown material A is drawn on the left-hand side, and material B is on the right-hand side. The interface where the connection matrix is given is artificial. It can be at z_0 or $z_0+\delta z$ as shown by the vertical solid and dashed lines, respectively. When the interface moves from z_0 to $z_0+\delta z$, the connection matrix will vary accordingly from $\mathbf{T}(z_0)$ to $\mathbf{T}(z_0+\delta z)$ as shown in Eq. (8).

If the interface is displaced by the distance of δz, and $|\delta z|\leq a$, the Taylor's expansions of the envelope function in material A can be written as

$$\psi_A(z_0+\delta z)=\psi_A(z_0)+\frac{d\psi_A}{dz}(z_0)\delta z+\frac{1}{2}\frac{d^2\psi_A}{dz^2}(z_0)\delta z^2+O(\delta z^3) \tag{3}$$

and

$$\frac{d\psi_A}{dz}(z_0+\delta z)=\frac{d\psi_A}{dz}(z_0)+\frac{d^2\psi_A}{dz^2}(z_0)\delta z+O(\delta z^2)\ . \tag{4}$$

In the formalism of the connection-matrix approach, it is assumed that, in each bulklike region, the variation of the envelope function within a lattice constant is negligible. Furthermore, in the tight-binding model, only the first derivative of the envelope function is retained in the derivation of the connection matrix.[5] Hence, the terms of second- and higher-order derivatives in Eqs. (3) and (4) can be ignored without increasing the degree of approximation. This results in the relation between the envelope function at z_0 and the envelope function at $z_0+\delta z$:

$$\begin{bmatrix}\psi_A(z_0+\delta z)\\ \nabla\psi_A(z_0+\delta z)\end{bmatrix}=\begin{bmatrix}1 & \delta\\ 0 & 1\end{bmatrix}\begin{bmatrix}\psi_A(z_0)\\ \nabla\psi_A(z_0)\end{bmatrix}, \tag{5}$$

where $\delta=\delta z/a$.

A similar relation can be established for material B:

$$\begin{bmatrix}\psi_B(z_0+\delta z)\\ \nabla\psi_B(z_0+\delta z)\end{bmatrix}=\begin{bmatrix}1 & \delta\\ 0 & 1\end{bmatrix}\begin{bmatrix}\psi_B(z_0)\\ \nabla\psi_B(z_0)\end{bmatrix}. \tag{6}$$

Therefore, when the interface is displaced to $z_0+\delta z$, the envelope function relation becomes

$$\begin{bmatrix}\psi_B(z_0+\delta z)\\ \nabla\psi_B(z_0+\delta z)\end{bmatrix}=\mathbf{T}(z=z_0+\delta z)\begin{bmatrix}\psi_A(z_0+\delta z)\\ \nabla\psi_A(z_0+\delta z)\end{bmatrix}, \tag{7}$$

with the connection matrix at $z_0+\delta z$,

$$\begin{aligned}\mathbf{T}(z=z_0+\delta z)&=\begin{bmatrix}1 & \delta\\ 0 & 1\end{bmatrix}\mathbf{T}(z=z_0)\begin{bmatrix}1 & \delta\\ 0 & 1\end{bmatrix}^{-1}\\ &=\begin{bmatrix}t_{11}+t_{21}\delta & t_{12}+(t_{22}-t_{11})\delta-t_{21}\delta^2\\ t_{21} & t_{22}-t_{21}\delta\end{bmatrix},\end{aligned} \tag{8}$$

where t_{11}, t_{12}, t_{21}, and t_{22} are the matrix elements of the connection matrix for the interface at z_0 as shown in Eq. (2). Equations (7) and (8) have been presented by Ando, Wakahara, and Akera in 1989.[5]

In this article, two methods will be suggested to examine the validity of the connection-matrix approach to quantum wells by using Eq. (8) and the numerical values of the connection matrix for the GaAs-$Al_xGa_{1-x}As$ interfaces given in Refs. 5 and 7. The first method is to reveal the dependence of the eigenenergy on the location of the interface. The second method is to demonstrate that the dependence is not entirely due to the change of the well width.

The first examination method is based on the upper schematic plot of the GaAs-$Al_xGa_{1-x}As$ quantum well in Fig. 2. For this quantum well, there are two interfaces located at z_1 and z_2 shown by the vertical solid lines in Fig. 2. The interface is artificial and it can be placed arbitrarily at any point between the interfacing atoms. For instance, the heterojunction at z_2 can have the interface at $z=z_2$ or at $z=z_2+\delta z$ as illustrated by the vertical dashed lines in the first model of Fig. 2, as long as $|\delta z|\leq a$.

Usually, z_2 is taken to be the location of the interface

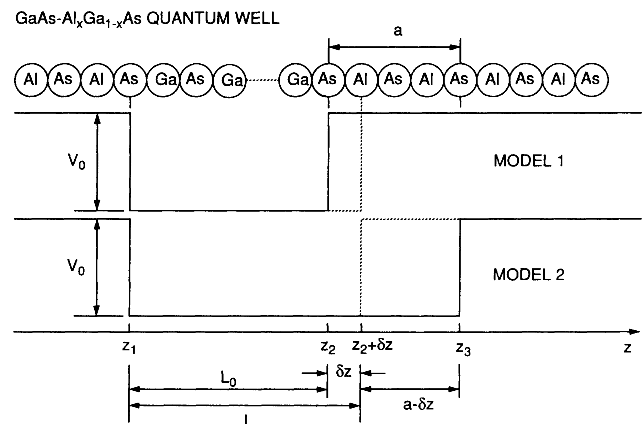

FIG. 2. Schematic plots of quantum-well models. The microscopic picture and two effective-mass models of the GaAs-$Al_xGa_{1-x}As$ quantum well are plotted. Model 1 is used for the first examination method, where the dependence of the eigenenergies on the interface location is studied. Models 1 and 2 have the same resultant well width, and are used for the second examination method to illustrate that the well-width change is not the only reason responsible for the eigenenergy dependence on the interface location.

where the connection matrix is given in the literature. For most of the physical applications of the connection matrix, the interface is simply taken to be at z_2. In this paper, moving the interface by δz is the method we suggest to investigate the consistency of the effective-mass model employing the connection matrix at the interface.

If the quantum well shown in the upper plot of Fig. 2 is to be modeled by the single-band effective-mass equation and the connection matrix at the interface, one can take the right-hand interface to be at either z_2 or $z_2+\delta z$. The well width of the quantum well should be taken as the separation between the locations of the two interfaces. Therefore, the model with the right-hand interface at $z_2+\delta z$ have the connection matrix given by Eq. (8) and the resultant well width of

$$L=L_0+\delta z \;, \tag{9}$$

where $L_0=z_2-z_1$ is the well width of the model with the right-hand interface at z_2.

The model with the two interfaces at z_1 and z_2 and the model with the interfaces at z_1 and $z_2+\delta z$ are simply two different simulations of the same physical system. They should produce the same confined electron levels in the quantum well if the effective-mass equation incorporated with the connection matrix is sufficient for this type of problem.

In the second examination method, the quantum well is simulated by two models. The first model has the well width of L_0 and the interface displacement of δz as shown in the upper plot of Fig. 2. The second model has the well width of L_0+a and the interface displacement of δz as shown in the upper plot of Fig. 2. The second model has the well width of L_0+a and the interface displacement of $-(a-\delta z)$ as shown in the lower plot of Fig. 2, where a is the lattice constant and $0\le\delta z\le a$ for this method. These two models have the same resultant well width of

$$L=L_0+\delta z=(L_0+a)+[-(a-\delta z)] \;.$$

If the eigenenergy dependence on the interface location revealed in the first examination method is simply due to the change of the well width, then the eigenenergies obtained by the two models of the second examination method should be identical. In Sec. III these two propositions will be inspected and the validity of the connection-matrix approach to quantum wells will be discussed.

III. RESULTS AND DISCUSSION

Both the effective-mass-dependent connection matrix proposed by Ando, Wakahara, and Akera[5] and the energy-dependent connection matrix proposed by Cuypers, and van Haeringen[7] will be examined by the two examination methods mentioned in Sec. II. Since the energy-dependent connection matrix is only available for the GaAs-AlAs interface in the work by Cuypers and van Haeringen, the GaAs-AlAs quantum well is used in the first examination method to compare the results predicted by the effective-mass-dependent and the energy-dependent connection matrices. It will be shown that the energy-dependent connection matrix does slightly better in the examination than the effective-mass-dependent connection matrix. But their results are not different enough for the major characteristics of the examination results to change.

The GaAs-AlAs quantum well has three quantum levels for the well width of about 100 Å. For the sake of simplicity in illustrations, a two-level GaAs-$Al_{0.3}Ga_{0.7}As$ quantum well will be employed after the comparison between the two connection matrices is completed. Hence, only the results obtained by the effective-mass-dependent connection matrix will be presented for the rest of the examinations.

The transfer-matrix method in Ref. 13 is modified to take the connection matrix into account. For the quantum-well model employing the energy-dependent connection matrix, self-consistent solutions for each quantum level are obtained by iterations. Hence, the results obtained in this section are analytic solutions.

The connection matrix of the GaAs-$Al_xGa_{1-x}As$ interface is given by

$$\mathbf{T}(\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As}\leftarrow\mathrm{GaAs})=\begin{bmatrix} t_{11} & t_{12} \\ t_{21} & t_{22}\end{bmatrix} . \tag{10}$$

The matrix elements t_{11}, t_{12}, t_{21}, and t_{22} obtained by the tight-binding model and the pseudopotential method will be given below.

The effective mass-dependent connection matrix proposed by Ando, Wakahara, and Akera is given at the As atom:[5]

$$t_{11}=\left[\frac{m(\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As})}{m(\mathrm{GaAs})}\frac{E_g(\mathrm{GaAs})}{E_g(\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As})}\right]^{1/2} , \tag{11}$$

$$t_{22}=\left[\frac{m(\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As})}{m(\mathrm{GaAs})}\frac{E_g(\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As})}{E_g(\mathrm{GaAs})}\right]^{1/2} , \tag{12}$$

and

$$t_{12}=t_{21}=0 \;. \tag{13}$$

In this paper, the band-gap energy, the effective mass, and the lattice constant of the $Al_xGa_{1-x}As$ crystal are taken to be

$$E_g(\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As})=\begin{cases}1.424+1.247x \quad (\mathrm{eV}) \\ 1.900+0.125x+0.143x^2 \quad (\mathrm{eV}) ,\end{cases} \tag{14}$$

$$m(\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As})=(0.067+0.083x)m_0 \;, \tag{15}$$

and

$$a(\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As})=5.6533+0.0078x \quad (\text{Å}) \;, \tag{16}$$

respectively.[14] For $x=1.0$ and 0.3, the connection matrix becomes

$$\mathbf{T}(\mathrm{AlAs}\leftarrow\mathrm{GaAs})=\begin{bmatrix}1.213 & 0 \\ 0 & 1.846\end{bmatrix} \tag{17}$$

and

$$T(Al_{0.3}Ga_{0.7}As \leftarrow GaAs) = \begin{bmatrix} 1.042 & 0 \\ 0 & 1.316 \end{bmatrix} , \quad (18)$$

respectively.

The connection matrix of the GaAs-AlAs interface calculated by Cuypers and van Haeringen is energy dependent and almost diagonal. The matrix element t_{11} can be taken as real, and t_{22} is almost real. As the energy changes from 0 to 1.5 eV, the matrix elements t_{11} and t_{22} vary from 0.92 to 0.9 and from 1.26 to 1.05, respectively. From Fig. 3 of Ref. 7, the dependence of t_{11} and t_{22} on the energy is almost linear for energy less than 0.9 eV. Therefore, the following linear relations are used in this paper, for 0 eV $\leq E \leq 0.9$ eV,

$$t_{11} = 0.92 - \left[\frac{0.02}{1.5} \right] E , \quad (19)$$

$$t_{22} = 1.26 - \left[\frac{0.21}{1.5} \right] E , \quad (20)$$

and t_{12} and t_{21} are the same as in Eq. (13), where E is the energy relative to the conduction-band minimum of GaAs. The location where the energy-dependent connection matrix is given is not mentioned in Ref. 7. This does not influence our work because the interface displacement is relative to the location where the numerical values of the connection matrices are normally given in the literature.

For the conduction band of the GaAs-$Al_xGa_{1-x}As$ quantum well, the connection matrix connects envelope functions of two s-symmetry bands. Hence, the connection matrix of the interface configuration obtainable by the mirror reflection of the interface configuration with the connection matrix of $\mathbf{T}_{BA}$ is computed by[5]

$$\mathbf{T}_{AB} = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \mathbf{T}_{BA}^{-1} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} . \quad (21)$$

The eigenenergies of the three quantum levels of the GaAs-AlAs quantum well are shown in Fig. 3. The results obtained by the effective-mass-dependent and the energy-dependent connection matrices are plotted in the solid and the dashed curves, respectively. The barrier height and the well width of the GaAs-AlAs quantum well are taken to be 446.6 meV (by assuming the conduction-band–offset ratio to be 0.6) and 101.7594 Å (36 monolayers of GaAs), respectively.

As the interface displaces from a to $-a$, the first, the second, and the third eigenenergies predicted by the effective-mass-dependent connection matrix deviate by 9.654, 33.691, and 56.428 meV, respectively; those predicted by the energy-dependent connection matrix deviate by 9.213, 32.549, and 54.637 meV, respectively.

The first examination method can also be formulated so that the displacement occurs at the interface at z_1 rather than at z_2. The computational results show that the eigenenergies as functions of the interface displacement relative to z_1 are the mirror reflection of Fig. 3 about $\delta z = 0$. Hence, we will concentrate on the examination on the heterojunction at z_2.

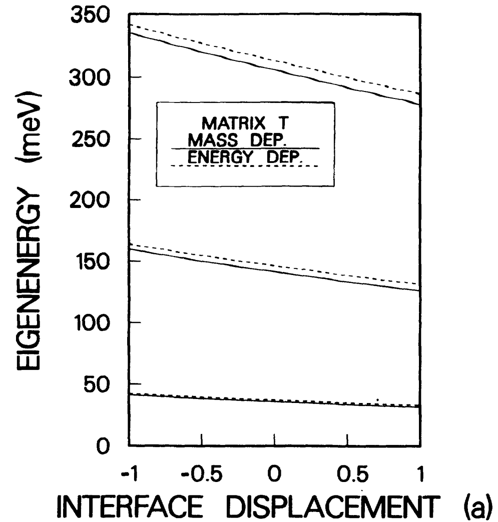

FIG. 3. Eigenenergies of the GaAs-AlAs quantum well. The eigenenergies of the three quantum levels of the GaAs-AlAs quantum well as functions of the interface displacement (in the unit of a lattice constant) are plotted. The barrier energy and the well width are 446.40 meV and 101.7594 Å, respectively. The solid and the dashed curves stand for the results obtained by the effective-mass-dependent and the energy-dependent connection matrices, respectively. The eigenenergy deviations due to the interface displacement are very close for both matrices.

To conclude, the energy-dependent connection matrix does slightly better in the examination than the effective-mass-dependent connection matrix. But the difference is too small to introduce significant change of the characteristics of the examination results. Therefore, for simplicity, we will, in the following discussions, focus on the examination on the two-level GaAs-$Al_{0.3}Ga_{0.7}As$ quantum well by using the effective-mass-dependent connection matrix.

The eigenenergies of the first and the second levels of the GaAs-$Al_{0.3}Ga_{0.7}As$ quantum well are shown in the lower and the upper subplots of Fig. 4, respectively. The barrier energy and the well width used in this figure are 224.46 meV and 101.7594 Å, respectively. The solid curves represent the physical solutions. Two nonphysical solutions are also plotted. The first one, denoted by the dashed curves, is the eigensolution obtained by holding the well width constant and varying the connection matrix as the interface displacement changes. The second one shown by the dotted curves is the eigenenergies obtained by holding the connection matrix unchanged and varying the well width. These two nonphysical solutions are presented to illustrate the effects of the well width and the connection matrix on the eigenenergies.

As mentioned in Sec. II, if the combination of the effective-mass equation and the connection matrix constitutes a sufficiently consistent model, the effects of the alteration of the connection matrix, as the interface moves, should compensate for the effects of the well width change. However, it is found that the effects of the well

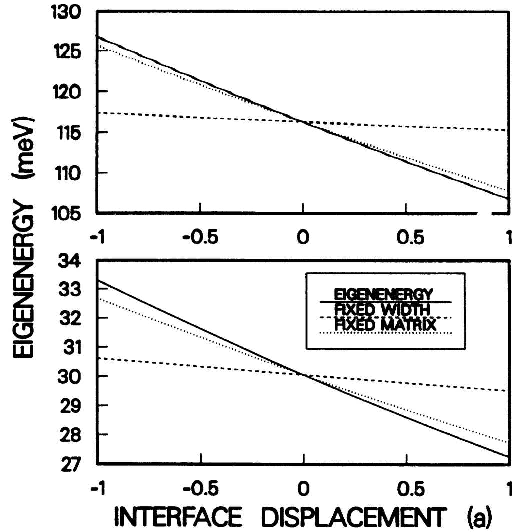

FIG. 4. Eigenenergies of the GaAs-$Al_{0.3}Ga_{0.7}As$ quantum well. The eigenenergies of the GaAs-$Al_{0.3}Ga_{0.7}As$ quantum well are plotted in solid curves. The barrier energy and the well width of the quantum well are 224.46 meV and 101.7594 Å, respectively. The nonphysical eigensolutions obtained by fixing the well width and by fixing the connection matrix are shown by the dashed and dotted curves, respectively. The eigenenergy deviation is dominated by the change of the well width.

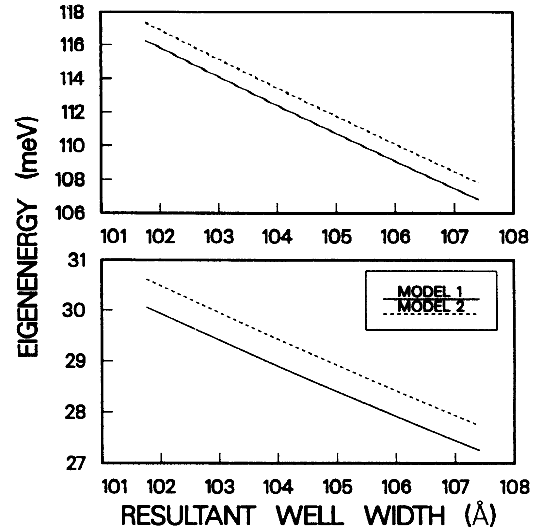

FIG. 5. Quantum wells with the same resultant well width. The eigenenergies of the two GaAs-$Al_{0.3}Ga_{0.7}As$ quantum-well models given in Fig. 2 are plotted versus the resultant well width. The results of models 1 and 2 are shown in the solid and dashed curves, respectively.

width and the effects of the connection matrix on the eigenenergies are in the same direction, and that the eigenenergy deviation is dominated by the variation of the well width. As the interface displacement changes from a to $-a$, the first and the second eigenenergies of the GaAs-$Al_{0.3}Ga_{0.7}As$ quantum well can differ by 6.058 and 19.948 meV, respectively.

The fact that the well-width change dominates the eigenenergy variation as the interface displaces is also responsible for the results (obtained for the GaAs-AlAs quantum well in Fig. 3) that eigenenergy deviations for the models employing the effective-mass-dependent and the energy-dependent connection matrices are rather close.

As the GaAs-$Al_{0.3}Ga_{0.7}As$ quantum well is simulated by the two models of the same resultant well width ($L_0+\delta z$) as sketched in Fig. 2, the eigenenergies of the first model with the well width of L_0 and the second model with the well width of L_0+a are shown as functions of the resultant well width L in Fig. 5 by the solid and the dashed curves, respectively. The lower and the upper subplots display the eigenergies of the first, and the second levels, respectively. In this figure the well width of the first model (L_0) is taken to be 36 monolayers (101.7594 Å). Hence, the well width of the second model (L_0+a) is 38 monolayers (107.4127 Å).

It is found that the eigenenergies predicted by the two methods with the same resultant well width are not identical. The differences are about 0.5 and 1 meV for the first and the second levels, respectively. These differences are small because, as pointed out in the first examination method, the energy deviation is dominated by the well-width change. The fact that they are not identical shows that the well-width change is not the only reason for the eigenenergy to deviate as the interface displaces.

As the Al composition in the barrier of the GaAs-$Al_xGa_{1-x}As$ quantum well varies from 0.2 to 0.45, the barrier height changes from 149.64 to 336.69 meV. The well width (L_0) is taken to be 36 monolayers. The eigenenergies obtained by $\delta z=0$, a, and $-a$ are shown in Fig. 6 by the solid, dashed, and dotted curves, respectively.

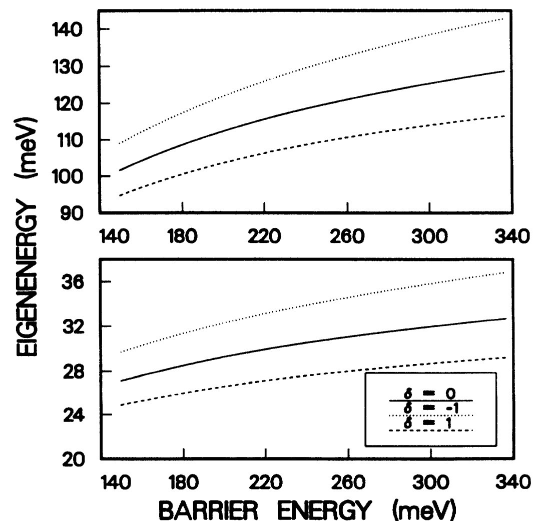

FIG. 6. Eigenenergy deviations versus barrier energy. The eigenenergies of the GaAs-$Al_xGa_{1-x}As$ quantum well as functions of the barrier energy are plotted in solid curves. The eigenenergies of the same system obtained by taking the interface displacement (δz) to be a and $-a$ are shown by the dashed and dotted curves, respectively.

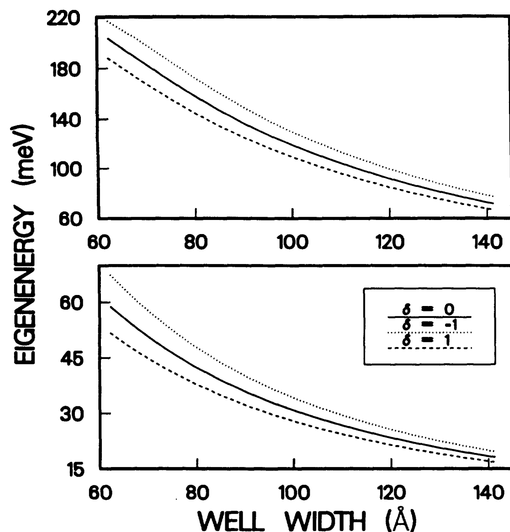

FIG. 7. Eigenenergy deviations versus well width. The eigenenergies of the GaAs-$Al_{0.3}Ga_{0.7}As$ quantum well as functions of the well width are plotted in solid curves. The eigenenergies of the same system obtained by taking the interface displacement (δz) to be a and $-a$ are shown by the dashed and dotted curves, respectively.

ly. The lower and upper subplots show the first and second eigenenergies, respectively. It is observed that the eigenenergy deviation due to a fixed interface displacement decreases as the barrier energy decreases.

In Fig. 7 the eigenenergies of the quantum well with the barrier energy of 224.46 meV are plotted as functions of the well width (L_0). The eigenenergies obtained by $\delta z=0$, a, and $-a$ are shown by the solid, dashed, and dotted curves, respectively. The eigenenergy deviations decreases as the well width increases. The trend that the eigenenergy deviation due to the interface displacement decreases as the barrier height decreases or as the well width increases is rather predictable because the effects of the well width overwhelm those of the connection matrix.

In this section it is shown that the GaAs-$Al_xGa_{1-x}As$ quantum-well model employing the single-band effective-mass equation and the connection matrix does not predict sufficiently consistent eigenenergies. In the connection-matrix approach to semiconductor heterojunctions, the wave functions on one side of the heterojunction are solved by assuming that the material on this side prevails in the entire space. The wave functions on the other side of the heterojunctions are obtained by the same assumption. Then, the wave functions are smoothly joined together at the interface to yield the connection conditions for the envelope functions.[5,7] The connection-matrix approach does not solve the heterojunction as a united system. In other words, it neglects the interaction between the materials on both sides of the heterojunctions. Hence, it is not surprising to see the inconsistent eigenenergies of the quantum well calculated by using the connection matrices obtained under the above assumptions.

IV. CONCLUSIONS

In this paper the connection-matrix approach to the GaAs-$Al_xGa_{1-x}As$ quantum wells is examined by varying the location of the interface between the interfacing atoms to observe the eigenenergy dependence on the location. As the interface is displaced between the interfacing atoms, the widths of the quantum well and the connection matrix alter accordingly. These two factors determine the eigenenergy of the quantum well. The effects of the two factors on the eigenenergies should cancel each other if the single-band effective-mass equation incorporated with the connection matrices at the heterojunctions is a sufficiently consistent model for the quantum well with abrupt heterojunctions.

Both the effective-mass-dependent and the energy-dependent connection matrices are explored. The results obtained from the GaAs-AlAs quantum well show negligible difference between the eigenenergy deviations calculated by the effective-mass-dependent and the energy-dependent connection matrices.

In this paper it is found that, as the interface displacement changes from a to $-a$, the first and second eigenenergies of the GaAs-$Al_{0.3}Ga_{0.7}As$ quantum well can deviate by about 6 and 20 meV, respectively. It is further verified that the deviations are dominated by the well width, but are not solely due to the change of the well width. Therefore, we conclude that the quantum-well model employing the single-band effective-mass equation and the connection matrices does not comprise a sufficiently consistent theoretical model. However, the eigenenergy deviations become less significant for the quantum well with smaller barrier energy and wider well width.

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