

## Optical properties of GaAs/AlAs superlattices with randomly distributed layer thicknesses

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Electronic states and optical properties of GaAs/AlAs superlattices with randomly distributed layer thicknesses are studied within the framework of the effective-mass approximation in the Wannier-Bloch mixing representation. By use of the improved Dean method, the energy spectra and envelope functions of the carriers in conduction and valence minibands are calculated for several samples with various degrees of randomness. From these results the optical-absorption coefficients of the transitions associated with several valence and conduction minibands are calculated as functions of the photon energy. It is found that the introduction of the randomness in the layer thicknesses gives rise to the reduction of the energy gaps. The calculated absorption edges shift to the infrared side and the intensities of several peaks in the absorption spectrum decrease.

### I. INTRODUCTION

Semiconductor superlattices and quantum wells have been studied extensively for several years. The electronic states and optical properties (including photoluminescence, photoabsorption, and light scattering) of these materials, especially of GaAs-Ga<sub>x</sub>Al<sub>1-x</sub>As multilayer structures, have been investigated experimentally and theoretically by many groups.<sup>1-12</sup> The theoretical models used for calculating the properties of the electronic states in such superlattices, in general, fall into two categories: those based on the tight-binding method, such as the empirical tight-binding treatment of Schulman and Chang,<sup>2</sup> and those based on the  $\mathbf{k}\cdot\mathbf{p}$  perturbation theory, such as the effective-mass approximation incorporating  $\mathbf{k}\cdot\mathbf{p}$  theory.<sup>3</sup> In recent literature it seems that the latter can sufficiently explain some of the optical properties of several semiconductor superlattices. In fact, the general features of the absorption spectra of these superlattices have been interpreted by using a simple effective-mass model, the "particle-in-a-box" model,<sup>13</sup> which assumes parabolic band structures for both the electrons and holes. The oscillator strengths for the band-to-band transitions are proportional to

$$F_{nn'} \equiv \langle f_n | g_{n'} \rangle \sim F_n \delta_{nn'},$$

where  $f_n$  and  $g_n$  are the envelope functions of the wave functions of the carriers in the  $n$ th conduction miniband and in the  $n$ th valence miniband, respectively. This means that the interband transition mainly occurs between a conduction state and a valence state having an identical principal quantum number with respect to the superlattice potential.

In the investigation of the optical properties, Sai-Halsz *et al.*<sup>14</sup> have reported a theoretical calculation for the ab-

sorption coefficients of semiconductor superlattices based on a simple envelope-function approximation (EFA). Such a calculation may predict the general features of the absorption spectrum, but it cannot explain several weak structures corresponding to the so-called forbidden transitions. A more realistic tight-binding model has been proposed by Chang and Schulman for semiconductor superlattice,<sup>2</sup> the miniband structures and optical properties have been calculated, and it is revealed that mixing of the heavy- and light-hole states in the superlattice potential can lead to the  $\Delta n \neq 0$  (forbidden) transitions.

At the same time, there has also been some interest in the study of the effect of disorder on superlattice properties. Dow, Ren, and Hess have presented theoretical calculations on the electronic structures of random superlattices.<sup>15</sup> Recently, the atomic-layer-doping technique— $\delta$ -doping—became a subject of numerous experimental studies. The reason that is, for this interest lies in the possibility that this doping may provide very high electronic sheet densities with enhanced low-field mobility in the superlattices of compound semiconductors. Betrum and Capasso<sup>6</sup> and Ihm *et al.*<sup>7</sup> have shown that the band structures of these superlattices can be greatly modified by inserting the  $\delta$ -doping layers into the well regions, as well as into the barrier regions of the superlattices. One of the novel features they observed is that the miniband widths are enhanced by introducing such  $\delta$ -doping layers. The physical origin of the experimental results can be partially explained by the calculations detailed in Refs. 7 and 8. More recently, superlattices with randomly distributed layer thicknesses have been fabricated, and the degree of randomness in the materials can be artificially controlled.<sup>9-11</sup> Experimental measurements on the photoabsorption and photoluminescence of these materials have revealed the optical properties to be quite different from those of bulk alloys and ordinary superlattices. It is

found that the optical-absorption edges of these random superlattices also shift to the long-wavelength side.

Until now there have been few theoretical studies on the properties of semiconductor superlattices with randomly distributed layer thicknesses. The randomness in the thicknesses breaks the periodic symmetry and the Bloch theorem is no longer valid. Wang *et al.*<sup>12</sup> have used a recursion method to calculate the local densities of states of an aperiodic semiconductor superlattice. As the method is numerically unstable in this calculation, only the smallest and largest eigenvalues are reliable, so one can hardly calculate the optical properties by this method.

In this paper we attempt to calculate the optical properties of GaAs/AlAs superlattices with randomly distributed layer thicknesses. Our motivation is that some unusual optical properties in these materials have been observed experimentally,<sup>9-11</sup> and this provides the possibility of producing some new materials with special optical properties by introducing this kind of randomness in the superlattices. Our purpose is to investigate the possible links between the physical properties and the structures of these materials, and to obtain results that can be compared with experiments. In dealing with the breaking of the periodic symmetry, we use a model based on the effective-mass approximation, but expressed by the Wannier-Bloch mixing representation with a Wannier tight-binding form in the growth direction and a Bloch form in the in-plane directions. In such a representation, the problem with a given in-plane momentum reduces to a disordered one-dimensional (1D) model in the tight-binding form. For such a 1D model, the energy spectrum and the envelope functions of the wave functions can be calculated by using an improved Dean method.<sup>16,17</sup> From these results, together with the  $\Delta n = 0$  selection rule, one can calculate the optical properties.

In Sec. II we describe the structural features of these materials. In Sec. III the Hamiltonian of the electronic system in the materials, expressed in the Wannier-Bloch mixing representation, is presented. In Sec. IV the energy spectrum and the envelope functions are numerically calculated by use of the improved Dean method. In Sec. V we give the procedure for determining the optical-absorption coefficients of the interband transitions and calculate, numerically, the optical-absorption spectrum of the transitions between the edges of the conduction and valence minibands. In Sec. VI we summarize the results and provide some concluding remarks.

## II. SUPERLATTICES WITH RANDOMLY DISTRIBUTED LAYER THICKNESSES

We consider a superlattice made from the alternating deposition of the layers of two compounds, GaAs and AlAs. If the superlattice has complete periodic symmetry, the layers are arranged as

$$\begin{array}{cccccccc} \text{GaAs} & \text{AlAs} & \text{GaAs} & \text{AlAs} & \text{GaAs} & \text{AlAs} & \cdots \\ L_A & L_B & L_A & L_B & L_A & L_B & \end{array},$$

where  $L_A$  ( $L_B$ ) is the thickness of layer GaAs (AlAs), so the system has a period of  $L_A + L_B$  in the growth direc-

tion. If the randomness in the layer thicknesses is introduced, the thickness of a special layer becomes a random variable. In the Wannier-Bloch mixing representation with a tight-binding form in the growth direction, the layer thickness only takes an integer value, which represents the number of the atomic planes within the layer. Thus, the distribution of the thicknesses can be expressed by the following stochastic functions:

$$P(L_A) = \sum_{i=1}^{N_A} p_{Ai} \delta(L_A - l_{Ai}), \quad (1)$$

$$P(L_B) = \sum_{i=1}^{N_B} p_{Bi} \delta(L_B - l_{Bi}),$$

with

$$\delta(l) = \begin{cases} 1, & l=0 \\ 0, & l \neq 0 \end{cases}$$

where  $l_{Ai}$  and  $l_{Bi}$  ( $i=1, 2, \dots, N_{A(B)}$ ) are the possible values of the thicknesses  $L_A$  and  $L_B$ , respectively;  $p_{A(B)i}$  is the probability of finding the thickness of a special layer of compound GaAs (AlAs) to equal  $l_{A(B)i}$ . It is obvious that

$$\sum_{i=1}^{N_A} p_{Ai} = 1, \quad \sum_{i=1}^{N_B} p_{Bi} = 1.$$

To generate a special thickness  $L_A$  or  $L_B$  according to this distribution, one can previously divide the range [0,1] into  $N_A$  or  $N_B$  intervals, and the length of the  $i$ th interval is proportional to  $p_{Ai}$  or  $p_{Bi}$ . Then, one can take a value  $x$  in the range [0,1] from a random-number generator. If  $x$  falls in the  $i$ th interval, then  $L_A$  or  $L_B$  assumes the value  $l_{Ai}$  or  $l_{Bi}$ . The entire superlattice is formed by alternate piling of GaAs and AlAs layers, with layer thicknesses produced in sequence from the above procedure. Thus, the layer thicknesses are randomly distributed, and the degree of the randomness is controlled by the values  $p_{Ai}$  and  $p_{Bi}$ . If

$$N_A = 1, \quad N_B = 1,$$

the randomness disappears and the periodicity of the superlattices is restored.

## III. THE HAMILTONIAN IN THE WANNIER-BLOCH MIXING REPRESENTATION

For the superlattices with randomly distributed layer thicknesses, the electrons and holes are free to move in the in-plane ( $x, y$ ) directions of the layers, whereas their motion along the growth direction is strongly affected by the potential discontinuities at the interfaces between the layers and by the randomness of the layer thicknesses. Owing to this randomness, there is no translational symmetry in the growth direction. Therefore, the Wannier-Bloch mixing representation exhibiting a Wannier form in the growth direction and a Bloch form in the in-plane directions is suitable. The basis functions of this representation can be denoted  $|\mathbf{k}_{\parallel} z\rangle$  where  $\mathbf{k}_{\parallel}$  indicates the in-

plane component of the momentum, and  $z$  is the coordinate of the wave function in the growth direction. These wave functions are related to the basis wave functions in the pure Wannier representation by the following transformation:

$$|\mathbf{k}_{\parallel}, z\rangle = N^{-1/2} \sum_{\mathbf{r}_{\parallel}} \exp(i\mathbf{k}_{\parallel} \cdot \mathbf{r}_{\parallel}) |\mathbf{r}_{\parallel}, z\rangle, \quad (2)$$

where  $|\mathbf{r}_{\parallel}, z\rangle$  is the atomic orbital at position  $(\mathbf{r}_{\parallel}, z)$ ,  $\mathbf{r}_{\parallel}$  is the coordinate in the  $x$ - $y$  plane, and  $N$  is the total number of the orbitals per  $x$ - $y$  plane.

The eigenstates of both the electrons and holes in the material can be expressed in terms of the linear combinations of these basis wave functions. We can write the state of the  $n$ th conduction miniband as

$$|\psi\rangle_{n, \mathbf{k}_{\parallel}}^e = \sum_z f_n(\mathbf{k}_{\parallel}, z) |\mathbf{k}_{\parallel}, z\rangle. \quad (3)$$

By substituting Eq. (2) into Eq. (3), one has

$$|\psi\rangle_{n, \mathbf{k}_{\parallel}}^e = N^{-1/2} \sum_{\mathbf{r}_{\parallel}, z} \exp(i\mathbf{k}_{\parallel} \cdot \mathbf{r}_{\parallel}) f_n(\mathbf{k}_{\parallel}, z) |\mathbf{r}_{\parallel}, z\rangle. \quad (4)$$

In the effective-mass approximation, the expansion coefficient  $f_n(\mathbf{k}_{\parallel}, z)$ , also known as the envelope function, satisfies the following equation:

$$\left[ \frac{\hbar^2}{2m_e(z)} \left( k_{\parallel}^2 - \frac{\partial^2}{\partial z^2} \right) + V_e(z) \right] f_n(\mathbf{k}_{\parallel}, z) = E_n^e(\mathbf{k}_{\parallel}) f_n(\mathbf{k}_{\parallel}, z), \quad (5)$$

where  $E_n^e(\mathbf{k}_{\parallel})$  is the eigenvalue of state  $|\psi\rangle_{n, \mathbf{k}_{\parallel}}^e$ ,  $V_e(z)$  is the superlattice potential, “seen” by the electrons, and  $m_e(z)$  is the effective mass of electrons in GaAs or AlAs, depending on where  $z$  is located. Because of the discontinuities of  $V_e(z)$  and  $m_e(z)$ , Eq. (5) should be solved with accompanying connection conditions at the interfaces. Owing to the randomness in the thicknesses, these connection conditions cannot be expressed in the same periodic form as that used in the study of the periodic superlattices. This creates an almost infinite number of connection conditions, which should be individually taken into account in solving the envelope functions. To deal with this difficulty, we introduce a tight-binding form of Eq. (5), which is more convenient than the continuous form in this case. This can be achieved by replacing the continuous media in Eq. (5) with a 1D lattice in the  $z$  direction, with site spacing  $d$ . Then, the coordinate  $z$  takes discrete values  $l$  ( $l$  being an integer), and the derivative in Eq. (5) becomes

$$\frac{\partial^2}{\partial z^2} f_n(\mathbf{k}_{\parallel}, z) = \frac{f_n(\mathbf{k}_{\parallel}, l+1) + f_n(\mathbf{k}_{\parallel}, l-1) - 2f_n(\mathbf{k}_{\parallel}, l)}{d^2}. \quad (6)$$

One can rewrite Eq. (5) as

$$\left[ \frac{\hbar^2}{2m_e(l)} \left( k_{\parallel}^2 + \frac{2}{d^2} \right) + V_e(l) - E_n^e(\mathbf{k}_{\parallel}) \right] f_n(\mathbf{k}_{\parallel}, l) - \frac{\hbar^2}{2m_e(l)d^2} [f_n(\mathbf{k}_{\parallel}, l+1) + f_n(\mathbf{k}_{\parallel}, l-1)] = 0. \quad (7)$$

It can be seen that Eq. (7) is actually a tridiagonal-matrix equation for a given  $\mathbf{k}_{\parallel}$ .

Similarly, the state of the  $m$ th valence miniband can be written as

$$|\psi\rangle_{m, \mathbf{k}_{\parallel}}^h = \sum_{\nu, \mathbf{r}_{\parallel}, z} \exp(i\mathbf{k}_{\parallel} \cdot \mathbf{r}_{\parallel}) g_m^{\nu}(\mathbf{k}_{\parallel}, z) |\mathbf{r}_{\parallel}, z\rangle, \quad (8)$$

where  $\nu = \frac{3}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{3}{2}$  is the quantum number of the valence subbands [ $\nu = \frac{3}{2}$  corresponds to the heavy-hole (hh) subband and  $\nu = \frac{1}{2}$  corresponds to the light-hole (lh) subband]. In the effective-mass approximation, the  $g_m^{\nu}$ 's satisfy the following equation:

$$\sum_{\nu'} [H_{\nu, \nu'}^h(\mathbf{k}_{\parallel}, z) + E_{m\nu}^h(\mathbf{k}_{\parallel}) \delta_{\nu, \nu'}] g_m^{\nu'}(\mathbf{k}_{\parallel}, z) + V_h^{\nu}(z) g_m^{\nu}(\mathbf{k}_{\parallel}, z) = 0, \quad (9)$$

where  $V_h^{\nu}(z)$  is the superlattice potential “seen” by the holes, the  $H_{\nu, \nu'}^h$ 's are the matrix elements of the Luttinger-Kohn Hamiltonian describing the bulk valence-subband structure,<sup>18</sup> and  $E_{m\nu}^h$  is the eigenvalue of the state. Because we focus only on the effect of randomness, at the first stage of the approximation we ignore the mixture of the heavy- and light-hole components, so the off-diagonal elements of the Luttinger-Kohn Hamiltonian vanish, and the four subbands ( $\nu = -\frac{3}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{3}{2}$ ) are decoupled. We can write the equation of the state in the  $\nu$ th subband as

$$\left[ \frac{\hbar^2}{2m_h^{\nu}(z)} \left( k_{\parallel}^2 - \frac{\partial^2}{\partial z^2} \right) + V_h^{\nu}(z) \right] g_m^{\nu}(\mathbf{k}_{\parallel}, z) = E_{m\nu}^h(\mathbf{k}_{\parallel}) g_m^{\nu}(\mathbf{k}_{\parallel}, z). \quad (10)$$

By using a procedure similar to that used for the conduction minibands, Eq. (10) can be transformed into the discrete form:

$$\left[ \frac{\hbar^2}{2m_h^{\nu}(l)} \left( k_{\parallel}^2 + \frac{2}{d^2} \right) + V_h^{\nu}(l) - E_{m\nu}^h(\mathbf{k}_{\parallel}) \right] g_m^{\nu}(\mathbf{k}_{\parallel}, l) - \frac{\hbar^2}{2m_h^{\nu}(l)d^2} [g_m^{\nu}(\mathbf{k}_{\parallel}, l+1) + g_m^{\nu}(\mathbf{k}_{\parallel}, l-1)] = 0. \quad (11)$$

For a given  $\mathbf{k}_{\parallel}$ , Eq. (11) is also a tridiagonal-matrix equation. In the next section we will solve these equations to obtain the energy spectrum and the envelope functions by use of the improved Dean method.

#### IV. ENERGY SPECTRUM AND ENVELOPE FUNCTIONS

In order to use the improved Dean method to solve the equations, we consider a finite sample with  $M$  sites in the

1D lattice of Eqs. (7) and (11), in which the random structure has been previously produced from the stochastic distribution of the layer thicknesses described in Eq. (1), and the values of the potential and mass at a given site are determined from the nature of the material where the site is located. For a given  $k_{\parallel}$ , the model becomes a 1D random chain. From the negative-eigenvalue theorem,<sup>17</sup> the number of states with eigenvalues less than  $E_n$  is simply the total number of negative  $u(i)$ 's, which are calculated from the following iterative relations:

$$u(i) = E(i) - E_n(k_{\parallel}) - \frac{t(i, i+1)t(i+1, i)}{u(i-1)}, \quad i = 2, \dots, M \quad (12)$$

$$u(1) = E(1) - E_n(k_{\parallel}), \quad (13)$$

where

$$E(i) = \frac{\hbar^2}{2m(i)} \left[ k_{\parallel}^2 + \frac{2}{d^2} \right] + V(i)$$

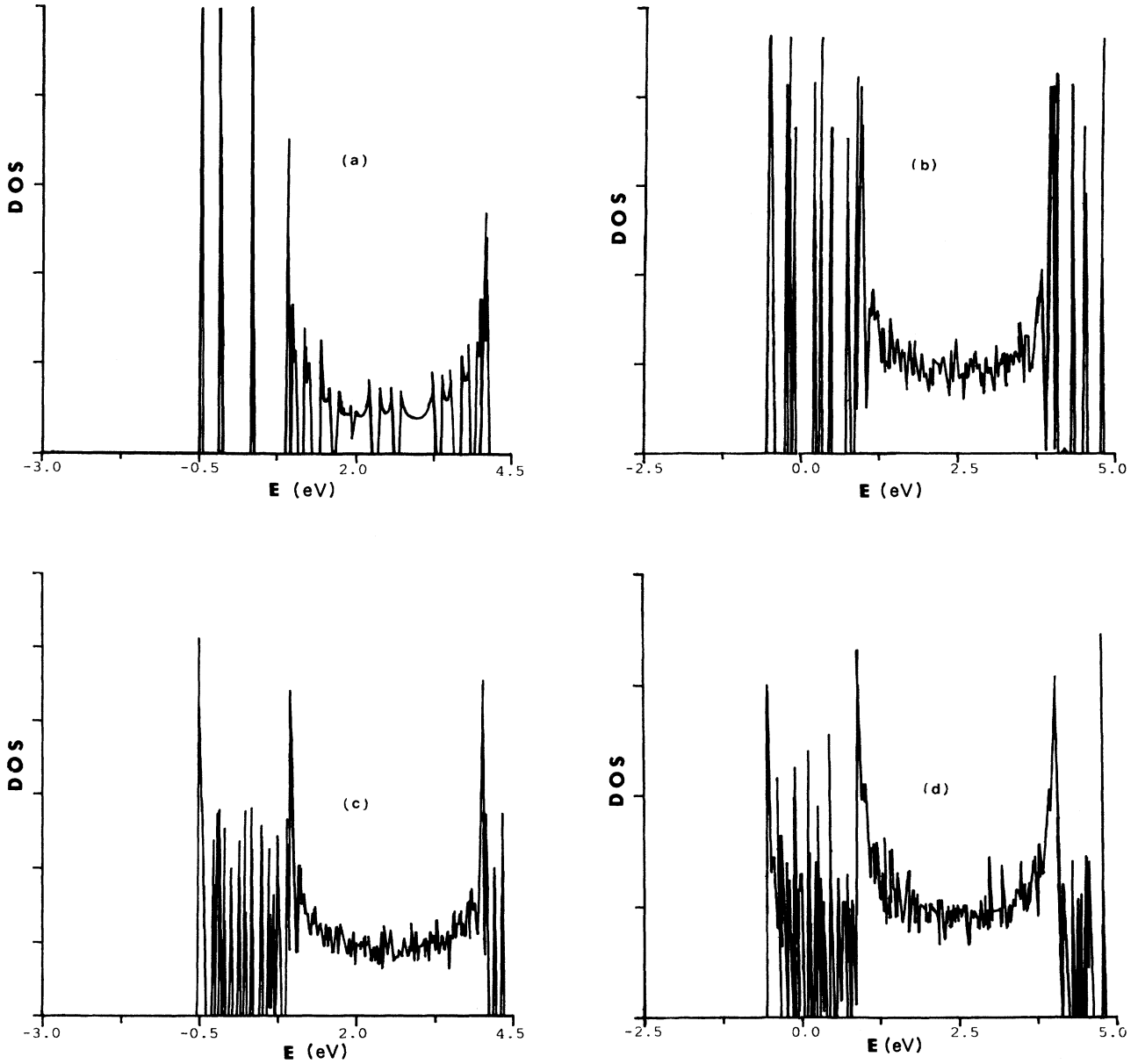


FIG. 1. Density of states (DOS) of conduction minibands with  $k_{\parallel} = 0$  in a finite system with 5000 sites in the  $z$  direction. The parameters in Eq. (1) are (a)  $N_A = N_B = 1$ ,  $p_{A_i} = p_{B_i} = 1$ , and  $l_{A_1} = l_{B_1} = 10$ ; (b)  $N_A = N_B = 3$ ,  $p_{A_1} = p_{B_1} = p_{A_3} = p_{B_3} = \frac{1}{10}$ ,  $p_{A_2} = p_{B_2} = \frac{4}{5}$ ,  $l_{A_1} = l_{B_1} = 9$ ,  $l_{A_2} = l_{B_2} = 10$ , and  $l_{A_3} = l_{B_3} = 11$ ; (c)  $N_A = N_B = 5$ , and  $p_{A_i} = p_{B_i} = \frac{3}{5}$  for  $i = 3$  and  $\frac{1}{10}$  for  $i \neq 3$ , where  $l_{A_i} = l_{B_i} = i + 7$ ; (d)  $N_A = N_B = 11$ , and  $p_{A_i} = p_{B_i} = \frac{1}{11}$  for  $11 \geq i \geq 1$ , and  $l_{A_i} = l_{B_i} = i + 4$ .

and

$$t(i, i \pm 1) = \frac{\hbar^2}{2m(i)d^2}.$$

Thus, one can obtain the densities of states for a given  $\mathbf{k}_{\parallel}$  for both the electrons and holes by use of this theorem.

After the energy spectrum is obtained, the improved Dean method described in Ref. 18 can be used to calculate the envelope functions. We denote the amplitude at site  $j$  of an eigenstate with eigenvalue  $E_n$  by  $a_j$ . If  $a_i \neq 0$ , we can choose  $a_i = 1$ , and the other amplitudes of the eigenstate can be obtained from the iterative relations:

$$a_{i \pm i'} = -t(i \pm i', i \pm (i' + 1)) \Delta_{i \pm i'}^{\pm} a_{\pm(i' - 1) + i} \quad \text{for } M \geq i \pm i' \geq 1, \quad (14)$$

and

$$\Delta_i^{\pm} = \frac{1}{[E(i) - E_n - t(i, i \pm 1)t(i \pm 1, i)\Delta_{i \pm 1}^{\pm}]}, \quad (15)$$

$$\Delta_M^+ = \frac{1}{E(M) - E_n}, \quad \Delta_1^- = \frac{1}{E(1) - E_n}. \quad (16)$$

From the definition, the 1D wave functions obtained from Eqs. (7) and (11) using this method are simply the envelope functions of the corresponding states in the conduction and valence minibands.

In our calculations the values of the parameters of GaAs and AlAs are chosen to be the same as those used in Ref. 19:

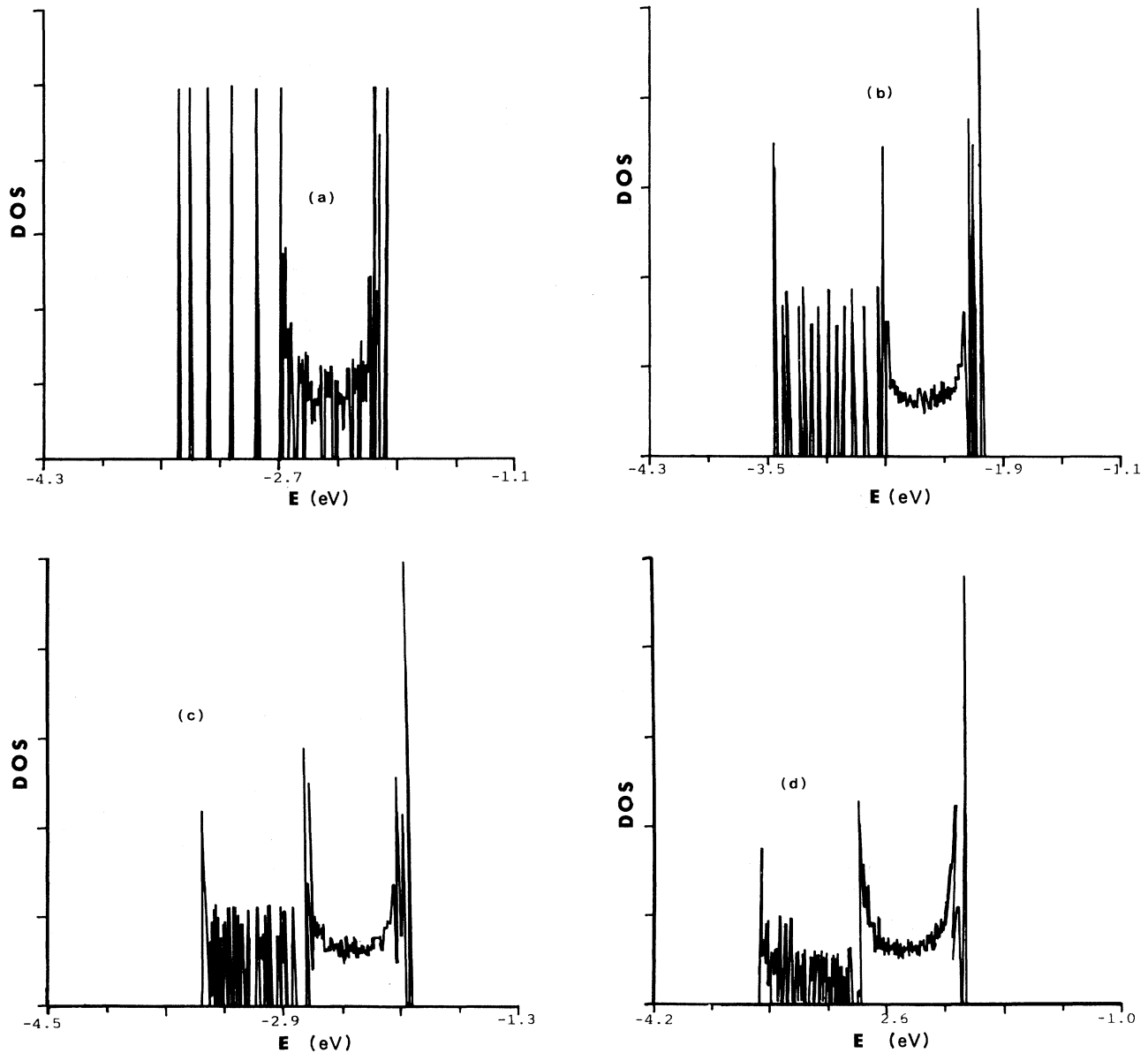


FIG. 2. Density of states of heavy-hole minibands with  $\mathbf{k}_{\parallel} = 0$  in a system with 5000 sites in the  $z$  direction. The parameters are the same as those of Fig. 1.

For GaAs:  $E_g = 1.43$  eV,  $m_{hh} = 0.34m_0$ ,  $m_{lh} = 0.09m_0$ ,  $m_e = 0.067m_0$ ,

For AlAs:  $E_g = 2.95$  eV,  $m_{hh} = 0.76m_0$ ,  $m_{lh} = 0.137m_0$ ,  $m_e = 0.15m_0$ .

(17)

The valence-subband offset of the superlattice potential is taken to be 40% of the difference in the band gap between bulk GaAs and AlAs; the conduction-subband offset is taken to be 60% of this difference.<sup>20</sup> The total number of sites in the 1D chain of Eqs. (7) and (11) is 5000. The energy spectrum is calculated for  $k_{\parallel} = 0$ . The densities of states of the electron minibands, heavy-hole minibands, and light-hole minibands are shown in Figs. 1, 2, and 3, respectively. The degree of the randomness in

the layer thicknesses is specified in the figure captions. It can be seen that when the degree of the randomness increases, the total widths of these minibands also increase, and the energy gap decreases. We also calculate the envelope functions of these minibands. From these results we can calculate the momentum matrix elements, the joint state densities of the conduction and valence minibands, and the optical-absorption coefficients.

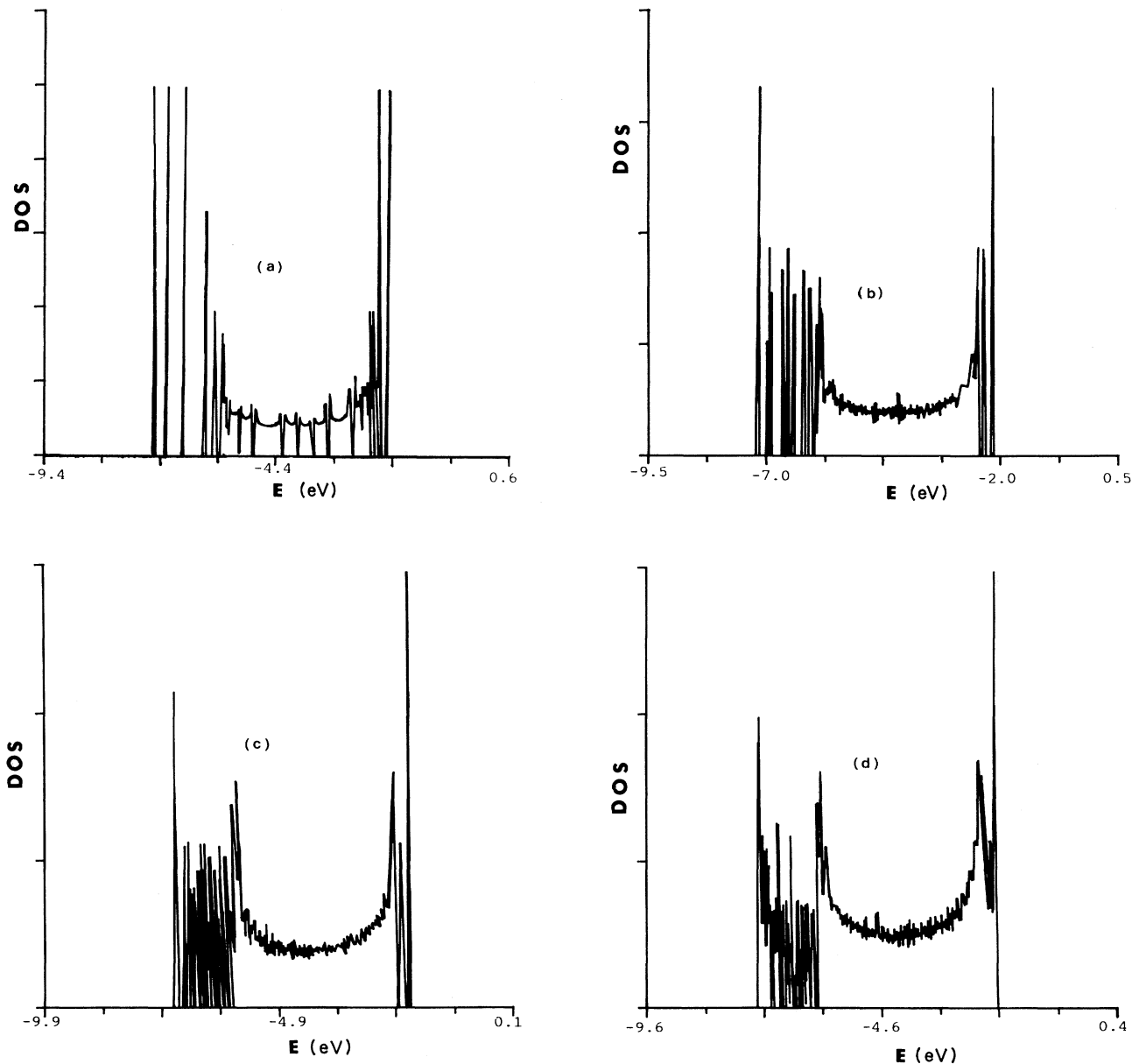


FIG. 3. Density of states of light-hole minibands in the same system as that depicted in Figs. 1 and 2.

### V. OPTICAL PROPERTIES

The optical property of concern here is photoabsorption from the interband transitions in the superlattices. The optical matrix elements obtained in the study of the absorption may also be useful for the analysis of the other optical properties, such as photoluminescence and photoconductivity.

Apart from a constant factor, the absorption coefficient of a superlattice can be written as<sup>2</sup>

$$\alpha(\hbar\omega) = (\hbar\omega)^{-1} \sum_{\mathbf{k}_{\parallel}, n, n'} |\hat{\mathbf{e}} \cdot \mathbf{P}_{nn'}(\mathbf{k}_{\parallel})|^2 \times \delta(E_{n'}(\mathbf{k}_{\parallel}) - E_n(\mathbf{k}_{\parallel}) - \hbar\omega), \quad (18)$$

where  $\hat{\mathbf{e}}$  is the unit vector in the direction of the light polarization, and where  $\mathbf{P}_{nn'}$  denotes the momentum matrix element between the eigenstate of the  $n$ th conduction miniband with energy  $E_n$  and the eigenstate of the ( $n'$ )th valence miniband with energy  $E_{n'}$ . In our model, the momentum matrix element  $\mathbf{P}_{nn'}$  can be expressed in terms of the coefficients  $f_n$  and  $g_{n'}$ , and in terms of the momentum matrix elements between the basis wave functions of the mixing representation:

$$\mathbf{P}_{nn'}(\mathbf{k}_{\parallel}) = \sum_{z, z', \alpha, \alpha'} f_n^*(\mathbf{k}_{\parallel}, z, \alpha) g_{n'}(\mathbf{k}_{\parallel}, z', \alpha') \times \langle \mathbf{k}_{\parallel}, z, \alpha | \mathbf{P} | \mathbf{k}_{\parallel}, z', \alpha' \rangle. \quad (19)$$

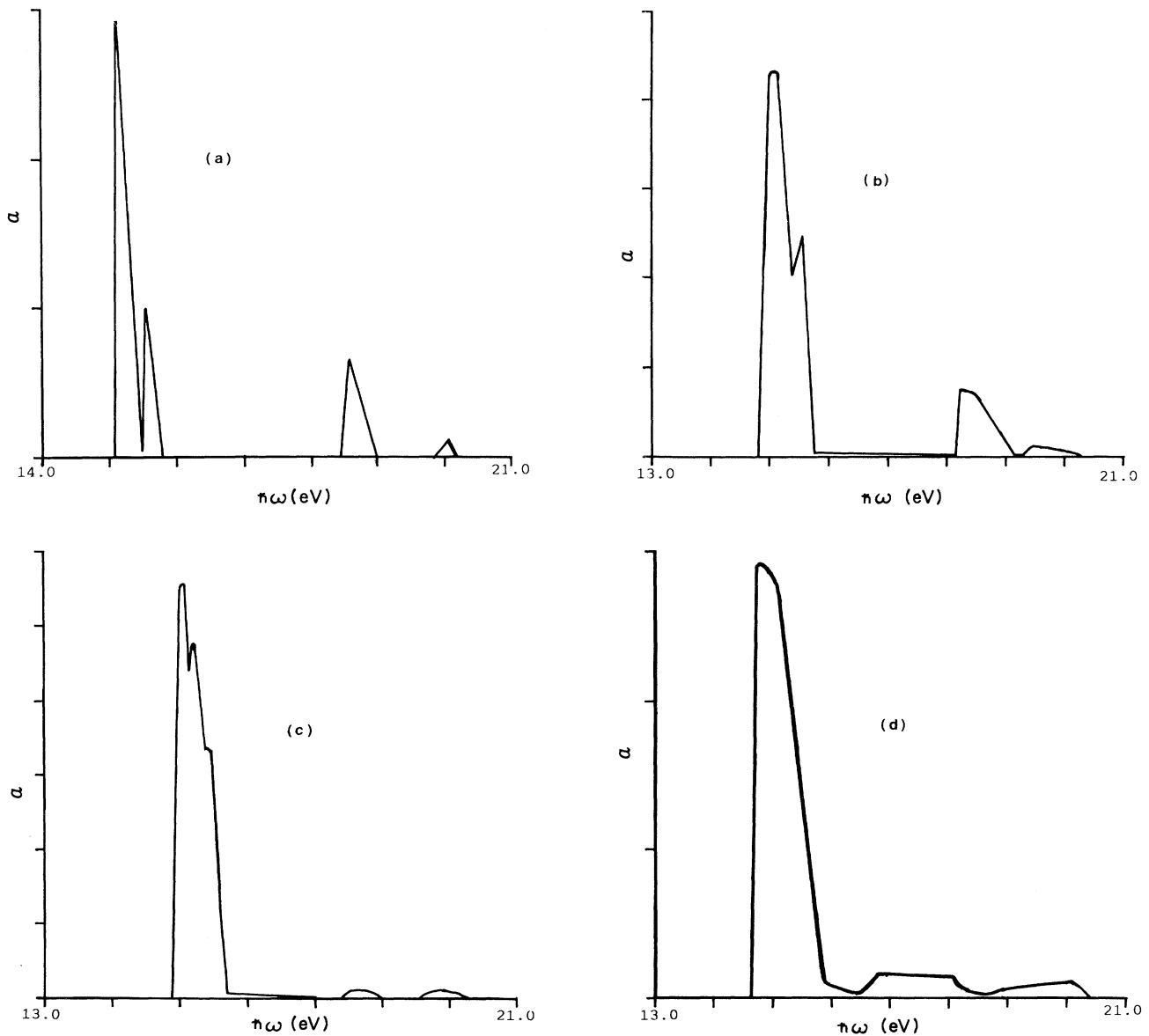


FIG. 4. Optical-absorption spectra for different degrees of randomness. The parameters of randomness are the same as those in Figs. 1(a)–1(d).

Because the atomic orbitals are sufficiently localized, and because the momentum matrix elements between the atoms separated by more than the first-nearest-neighbor distance can be neglected, the matrix element  $\langle \mathbf{k}_{\parallel}, z, \alpha | \mathbf{P} | \mathbf{k}_{\parallel}, z', \alpha' \rangle$  is not much affected by the interfaces of the superlattice, and is almost the same as that of the bulk semiconductors, as has been illustrated in Ref. 21.

In this paper we only consider the absorption from the transitions between the miniband edges to estimate the effect of the randomness in the layer thicknesses. This means that only the contributions from the states with  $\mathbf{k}_{\parallel} = 0$  are taken into account. The absorption coefficient then reads

$$\alpha(\hbar\omega) = (\hbar\omega)^{-1} \sum_{n, n'} |\hat{\mathbf{e}} \cdot \mathbf{P}_{nn'}(0)|^2 \rho_{nn'}(\hbar\omega), \quad (20)$$

where  $\rho_{nn'}(\hbar\omega)$  is the joint density of states associated with the  $n$ th conduction miniband and the  $(n')$ th valence miniband. This approximate expression for the absorption has often been used in the literature, and it may give a reasonable schematic description of the absorption spectrum.

The selection rules for the transitions caused by incident light with a given polarization can also be established. For light polarized in the  $z$  direction, only the transitions associated with the light-hole and conduction states are possible, whereas for light polarized in the  $x$  or  $y$  direction the transitions associated with the conduction states and either of the light- or heavy-hole states are possible. In the present calculation we assume that the polarization vector is parallel to the  $x$  direction. In this case the oscillator strength related to the momentum matrix element between the heavy-hole and conduction states is three times that of the element between the conduction and light-hole states; this has been investigated from the standpoint of the symmetry of these spin-orbit-coupled states of the valence band.<sup>2</sup>

The optical-absorption spectra obtained for different degrees of randomness are shown in Fig. 4. In our calculation it is also found that the main contribution to the absorption comes from those interband transitions that obey the  $n = 0$  selection rule. In fact, the superlattice po-

tentials “seen” by the electrons and holes have the same random structure; thus, the wave functions of an electron and a hole with the same principal quantum number have almost the same spatial structure, and are mostly overlapping. Therefore, the contribution from the transition between these states is enhanced. This is just a unique structural feature of this type of randomness. Another result that can be seen from Fig. 4 is that, when the degree of randomness increases, the peaks in the absorption spectrum become lower, and the absorption edge shifts to the long-wavelength side.

## VI. SUMMARY

We have investigated the electronic states and optical properties of semiconductor superlattices with specially constructed randomness—randomness in the layer thicknesses. The Hamiltonian in an effective-mass model has been expressed in the mixed representation with a tight-binding form in the  $z$  direction and with a Bloch form in the  $x$  and  $y$  directions. Thus the model reduces to a 1D lattice for a given  $\mathbf{k}_{\parallel}$ , and the energy spectrum and the envelope functions of the states can be obtained using the improved Dean method. The absorption spectrum has been calculated via use of a simplified scheme. The calculations have been done for several samples with different degrees of randomness. Upon comparing the results for different samples, it can be seen that, when the degree of randomness increases, the energy ranges of the minibands are widened, the energy gap decreases, the optical-absorption peaks become lower, and the absorption edges shift to the long-wavelength side. These results are in qualitative agreement with experiments.<sup>9–11</sup> The unique structural feature of this type of randomness may make it possible to invent some new optical or electrical devices.

## ACKNOWLEDGMENTS

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