Symmetry-dependent localization in a finite superlattice

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Effects of fluctuations in layer thickness on the electronic properties of a semiconductor superlattice have been investigated. It is shown that the degree of localization associated with fluctuations in the well widths depends on the symmetry of the system, i.e., the electronic states are more likely to be localized in the system with lower symmetry. It is also shown that while, in general, broken symmetry leads to localization, extended states also arise in certain nonsymmetric systems. In addition, there always arise strongly localized states at the sites of perturbed wells whose energies lie in the band-gap region. The energies of these states are observed to be independent of system size. Slight fluctuations in the barrier widths, in contrast to those in the well widths, cause neither significant changes nor any localization tendency in the electronic states.

I. INTRODUCTION

In recent years, there have been numerous investigations, both experimental and theoretical, to understand the physics of electronic transport and the localization properties in semiconductor superlattices (SL's). Among them, several examples are studies on intentionally disordered SL's,[1,2] electric-field-induced localization,[3–5] the origin of negative resistance,[6–8] the quantized Hall effect,[9] and surface states in SL's,[10,11] etc. One of the fundamental problems we often meet in real situations is the effects of slight fluctuations in layer thicknesses in SL's. In an ideal semiconductor SL, consisting of completely periodic potentials, the electronic states are extended Bloch waves with their energies distributed in minibands due to the coupling between wells which arises from resonant tunneling through the thin barriers. In a real situation, however, deviations from perfect periodicity caused, e.g., by slight fluctuations in layer thickness, alter the coupling and can induce a degree of localization. The investigations done by Littleton and Camley[12] sought to demonstrate, through the model calculation of a ten-period SL, that these fluctuations result in localization of electronic states instead of delocalized Bloch waves. These rather surprising results stimulated our interest to further investigate localization properties under such fluctuations.

In this paper, we show that the degree of localization in the electronic states depends, among other things, on the symmetry of the system, and the arguments of Littleton and Camley are not generally true. While electronic states are more likely to be localized in the system containing less symmetry, under certain conditions, it is shown that, even in nonsymmetric cases, some of the eigenmodes of Bloch states remain unchanged and nonlocalized while others change and become localized.

Whenever there are fluctuations in the well widths, there always exist strongly localized states in the perturbed well, whose energies lie in the band-gap region. These energies are observed to be independent of the system size but depend solely on the degree of fluctuations and the SL parameters. Our methods are essentially the same as those of Littleton and Camley,[12] although our calculation method is less complex. Of the systems investigated with different SL sizes, only the data pertaining to a nine-period SL are presented here as a typical example.

II. METHOD

The potential of the investigated superlattice consists of nine rectangular wells. The material parameters were chosen to be those appropriate for $In_{0.754}Ga_{0.246}As_{0.536}P_{0.465}/InP$.[13] For this structure, the height of the barriers between wells is 253 meV; the effective masses m_1^* and m_2^* for wells and barriers are $0.059m_e$ and $0.080m_e$, respectively. The widths of an original superlattice, w and b, are taken to be 100 and 50 Å for wells and barriers, respectively. The wave functions in the wells can be written as

$$\psi_N = A_N e^{ik_1[x-(N-1)d]} + A_N' e^{-ik_1[x-(N-1)d]} \quad \text{for the } N\text{th well}, \tag{1}$$

where d is the period of a superlattice and $k_1 = (2m_1^* E)^{1/2}/\hbar$ is the wave number in the wells. The wave-function coefficients A_N and A_N' are complex conjugates of each other and are determined using the effective-mass Hamiltonian and Bastard's boundary conditions,[14] which take into account effective-mass jumps. The coefficients A_2 and A_2' can be written in terms of A_1 and A_1' using the transfer matrix $\underline{M}$:

$$\begin{bmatrix} A_2 \\ A_2' \end{bmatrix} = \underline{M} \begin{bmatrix} A_1 \\ A_1' \end{bmatrix} , \tag{2}$$

where

$$\underline{M} = \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix} . \tag{3}$$

General properties of matrix $\underline{M}$ are $\det\underline{M}=1$, $M_{11}=M_{22}^*$, and $M_{12}=M_{21}^*$.[15] If the origin of our coordinate system is taken to be the left end of the first well, we can write

$$M_{11}=\exp(ik_1 w)\left\{\cosh(k_2 b)+i\frac{K-K^{-1}}{2}\sinh(k_2 b)\right\} ,$$

$$M_{12}=-\exp(-ik_1 w)i\frac{K+K^{-1}}{2}\sinh(k_2 b) ,$$

where k_2 is the wave number in barriers and K is the wave-number ratio defined as

$$k_2=\frac{[2m_2^*(V-E)]^{1/2}}{\hbar} , \tag{4}$$

$$K=\frac{k_1 m_2^*}{k_2 m_1^*} . \tag{5}$$

When the superlattice is perfectly periodic, we can represent

$$\begin{bmatrix} A_N \\ A_N' \end{bmatrix} = \underline{M} \begin{bmatrix} A_{N-1} \\ A_{N-1}' \end{bmatrix} \tag{6}$$

and

$$\begin{bmatrix} A_9 \\ A_9' \end{bmatrix} = \underline{M}^8 \begin{bmatrix} A_1 \\ A_1' \end{bmatrix} .$$

However, if there are fluctuations in the layer widths, Eq. (6) is not generally true and more than one transfer matrix must be used in order to connect A_9 with A_1. Finally, eigenenergies and eigen-wave-functions are found by enforcing matching conditions at both ends of a superlattice:

$$\frac{A_1'}{A_1}=\frac{K+i}{K-i} , \tag{7}$$

$$\frac{A_9'}{A_9}=\frac{\exp(ik_1 L)(1+iK)}{\exp(-ik_1 L)(1-iK)}=-\exp(i2k_1 L)\frac{A_1}{A_1'} , \tag{8}$$

where L is the total length of the superlattice and A_1' (A_9') is the complex conjugate of A_1 (A_9). In general, there exist N solutions in each miniband for an N-period superlattice.

III. RESULTS

The above method was first applied to the nine-period superlattice with perfect periodicity. Eigenenergies and corresponding wave functions squared for the first miniband are depicted in Fig. 1. The second miniband appears in the region of energy 126.14–138.25 meV. Electronic states are completely delocalized indicating Bloch waves, as shown in Fig. 1. Although not shown here, the overall pattern of the wave function squared in the second miniband is similar to that of the first miniband except for the fact that one node exists in each well. As the number of wells in the superlattice increases, miniband width is expected to increase and approach the values of an infinite superlattice, i.e., 32.60–34.76 meV and 125.86–138.60 meV for the first two bands, respectively, while the center of each band corresponds approximately to the eigenvalue of an isolated quantum well and, thus, remains almost unchanged.

Figure 2 presents a case identical to that of Fig. 1 except the fifth well is widened by Δ (=5 Å) while Figs. 3 and 4 display eigenmodes for the lowest and the second lowest minibands, respectively, where both the fourth and the seventh wells are widened by 5 Å compared to the original superlattice (Fig. 1). Except for the lowest-energy mode (hereafter denoted as the LS mode, where LS denotes localized state), the remaining modes in Fig. 2 remain extended states. Momentarily, let us ignore LS modes in the following discussions. In Fig. 2 the central symmetry of the potential is maintained and the localization of the electronic states to one side of the perturbed well is prohibited by the law of parity conservation. However, if we consider the ten-period superlattice in which the fifth well is widened by Δ compared to the other wells, as shown in Fig. 6 of Ref. 12, no such symmetry

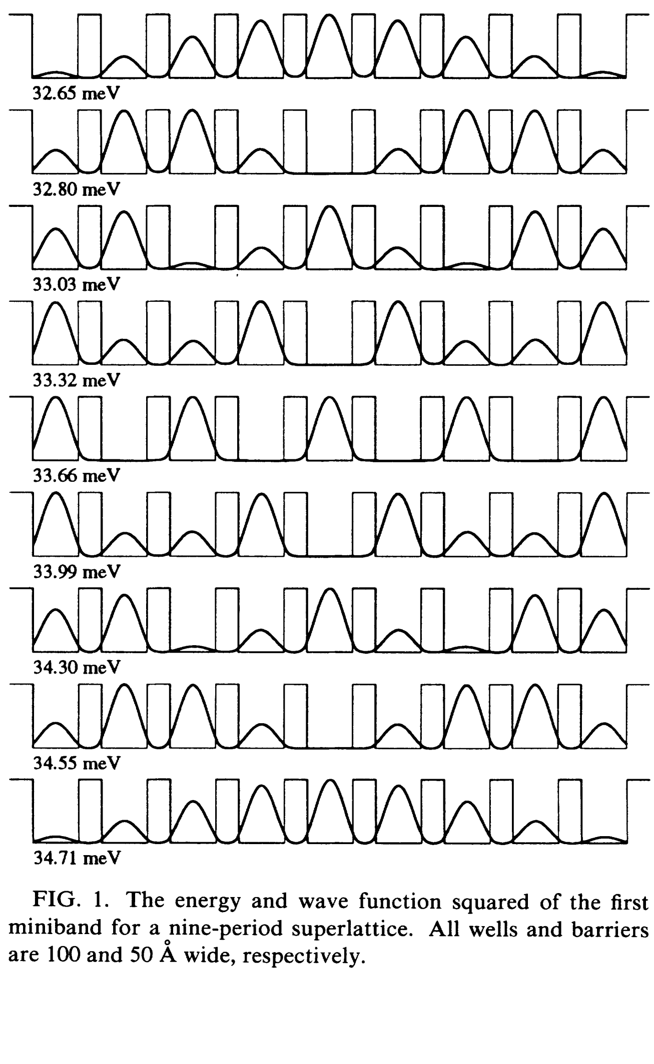

FIG. 1. The energy and wave function squared of the first miniband for a nine-period superlattice. All wells and barriers are 100 and 50 Å wide, respectively.

exists and wave functions are all localized on either the left- or right-hand side of the perturbed well. Thus, in the latter case, one would say that the perturbed well acts like an extremely large barrier, greatly reducing the coupling between the opposite sides (with respect to the perturbed well) of the superlattice. This observation of the symmetry-dependent localization in the electronic states is further confirmed in Figs. 3 and 4. The two lowest modes in Fig. 3 (Fig. 4) correspond to LS modes near the first (second) band. Except for the LS modes, all the modes are localized in either the first three wells or the last five wells. This interesting pattern can be explained as follows. Since a perturbed well acts like a nearly infinite barrier in a nonsymmetric potential, one can separate the two opposite sides of the fourth well. We then see that local symmetry holds for the potential of the last five wells and, thus, no further localization occurs. Thus, it becomes apparent that well-width perturbations which preserve symmetry, globally or locally, fail to produce localization.

Another interesting observation is the fact that even modes in Fig. 2 have the same energies and wave functions as the corresponding modes in Fig. 1. After careful examination of this and other such cases, our observations lead us to the following general conclusion: when there exist eigenmodes such that the probability of finding the electron in the ith well is zero, perturbation of the ith well width has a negligible effect on these special modes. For a ten-well superlattice, no such mode exists[16] and, thus, all the eigenmodes change with fluctuations in the layer widths. The same phenomenon can be observed in the case in which the seventh well is widened by 5 Å in a nine-well superlattice. In this case, since there exists neither symmetry nor the exceptional case of zero probability of electrons in the seventh well, all the modes (except LS modes) are localized on either side of the seventh well with their energies different from those in Fig. 1. In contrast, Fig. 5 shows a nine-well superlattice identical to Fig. 1 except the sixth well is widened by 5 Å. Since the probability of finding electrons in the sixth well is zero for the fifth mode, an interesting case arises. The fifth mode ($E=33.66$ meV) in Fig. 5 is seen to be completely identical to the fifth mode in Fig. 1, indicating the existence of an extended Bloch wave even under conditions of no symmetry. The remaining modes follow the general pattern explained in the preceding paragraph, showing localized states rather than Bloch waves.

Now, let us turn to the discussion of LS modes. When one of the wells in a superlattice is widened by 5 Å, two LS modes are found at the energies of 31.14 (see Fig. 2) and 121.52 meV regardless of the position of the perturbed well (except for end wells) and of the size of the superlattice (number of wells). The main reason is that LS modes are strongly localized at the site of the perturbed well and are closely related to the eigenvalues of an isolated well. The eigenvalues of a single quantum

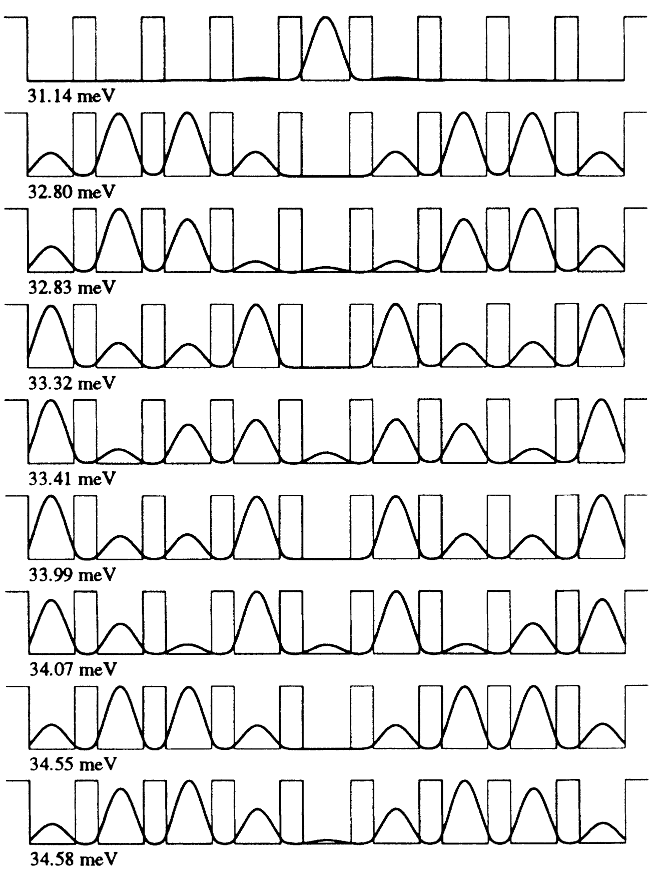

FIG. 2. Same as Fig. 1, except the fifth well is widened by 5 Å.

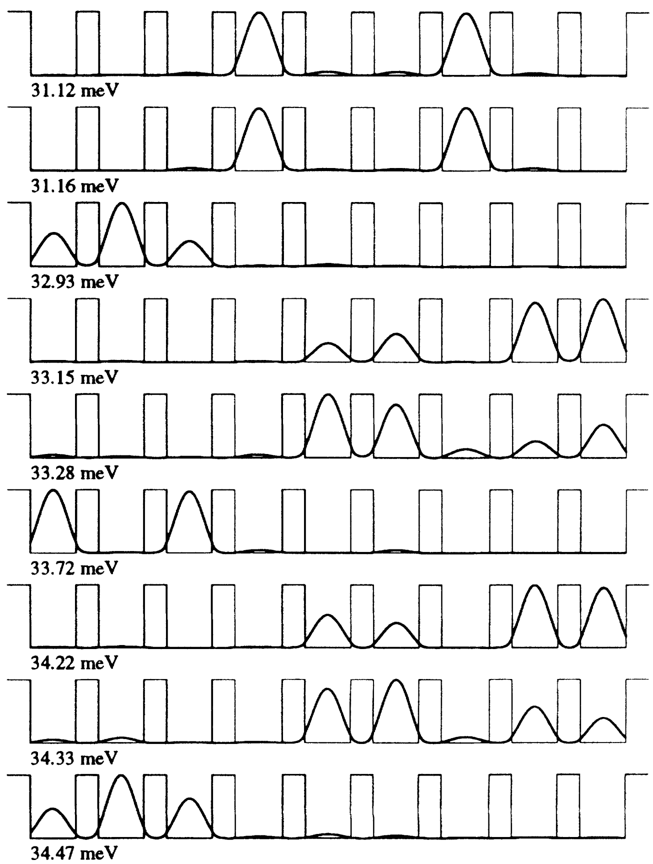

FIG. 3. Same as Fig. 1, except the fourth and the seventh wells are widened by 5 Å.

well bounded by barriers of height V can be written as[17]

$$\tan[k_1 w/2] = K^{-1} \quad \text{even} , \tag{9}$$

$$\cot[k_1 w/2] = -K^{-1} \quad \text{odd} , \tag{10}$$

where K is defined in Eq. (5). The values from Eqs. (9) and (10) are 31.36 and 123.07 meV, which are close to, but different from, the energies of the LS modes. From further observations of the effects of variation in the well width and by examining the case of an infinite superlattice,[18] the following statements can be made.

(i) Fluctuations in the well width always produce strongly localized states (LS modes) whose energies lie in the band-gap region. Outside the perturbed well, their wave functions decay exponentially in an oscillating pattern.[18] As Δ increases, they decay more sharply.

(ii) Energies of LS modes are close to eigenvalues of an isolated quantum well (of width $w+\Delta$), but are further removed from the energy bands than the latter due to the interaction with neighboring wells. They are independent of the size of the superlattice.

(iii) The miniband widths for a finite superlattice are decreased slightly by the introduction of fluctuations in the layer thicknesses. However, as the system becomes larger, this effect is less observable.

(iv) Slight fluctuations in the barrier widths, in contrast to those in the well widths, cause neither any significant changes in the eigenmodes nor any localization tendency, even when barrier widths approach the penetration depth.

We emphasize that statement (ii) is even true for negative Δ. As an example, when $\Delta = -5$ Å, the lowest LS mode is located between the first and second bands and has an energy of 36.49 meV while the solution from Eq. (9) is 36.25 meV.

Under fluctuations of several layers, i.e., as shown in Fig. 3, the LS mode ($E = 31.14$ meV) in Fig. 2 now splits into two states ($E = 31.14 \pm 0.02$ meV), i.e., symmetric and antisymmetric, with respect to the center of the two perturbed wells. This energy splitting originates from the coupling between the two perturbed wells through the tunneling effect. Similar, but rather large energy splitting of LS modes can be observed in the second miniband ($E = 121.5 \pm 0.2$ meV), as shown in Fig. 4. As the distance between two perturbed wells becomes larger, the coupling and, therefore, the energy splitting decrease.

In conclusion, we have investigated the effect of fluctuations in layer thickness on the electronic properties of a superlattice. One of the profound effects thus observed is the symmetry-dependent localization, along with the existence of LS modes. It is found that well-width perturbations that preserve symmetry, globally or locally, fail to produce localization. When there exist eigenmodes such that the probability of finding the electron in the ith well is zero, a perturbation in the ith well width has a negligible effect on these special modes. In addi-

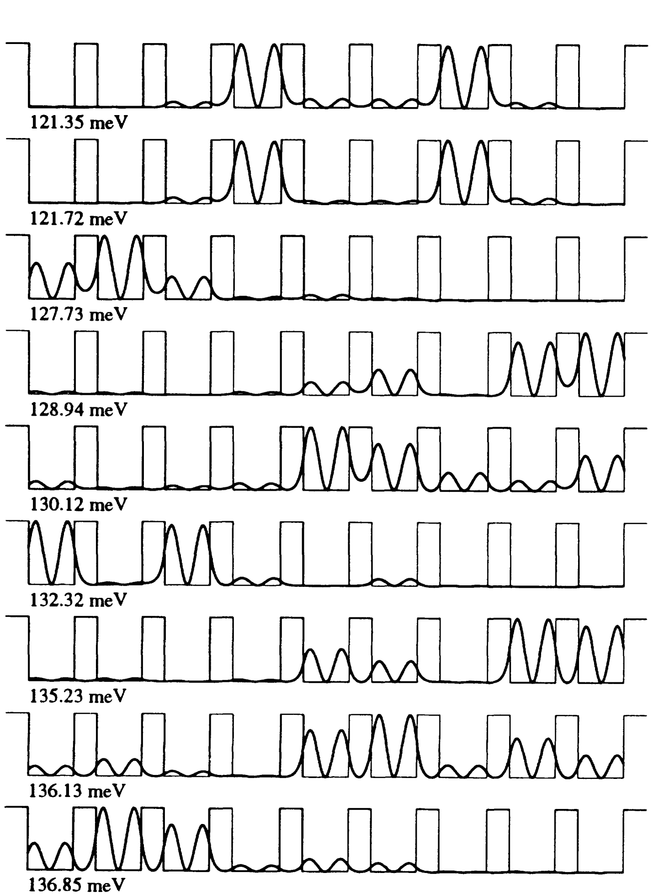

FIG. 4. Same as Fig. 3, except for the second miniband.

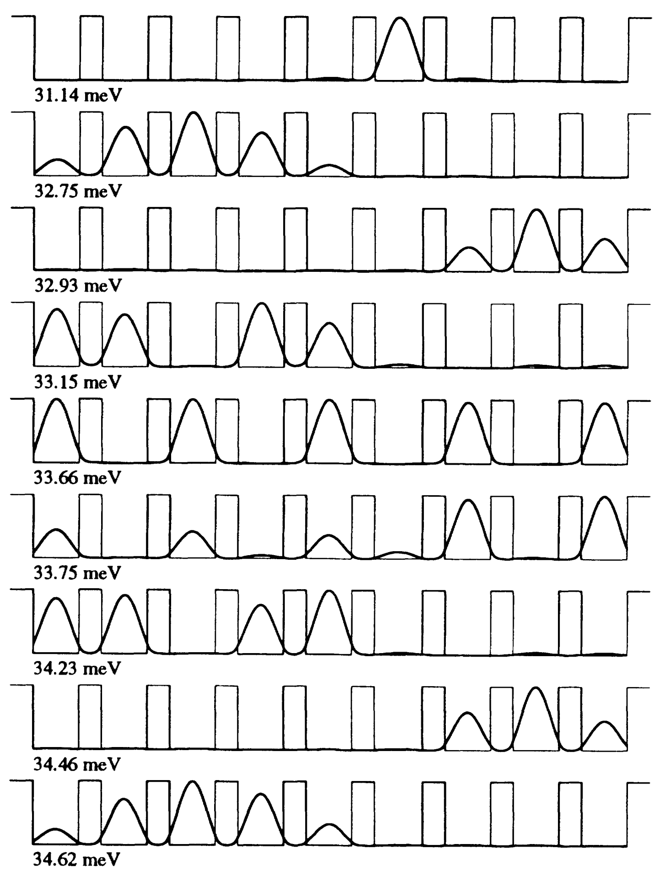

FIG. 5. Same as Fig. 1, except the sixth well is widened by 5 Å.

tion, details of the properties of LS modes are summarized in the four statements given in this section.

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