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Intersubband Transitions in an Asymmetric Quantum Well with a Thin Barrier of a Delta-Function Potential

by

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**Intersubband transitions in an asymmetric quantum well
with a thin barrier or a delta-function potential**

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The changes in the bound-state energies and oscillator strength for intersubband transitions brought about by a thin barrier in the middle of an asymmetric quantum well are calculated, with a particularly close look at such changes as the middle barrier height approaches the bound-state energies. It is found that the oscillator strength goes through a slight change as the barrier height approaches the ground-state energy but an abrupt change when it approaches the excited bound-state energy. A suitable explanation for this change is provided. A similar tailoring of the intersubband transitions is also achieved by placing a delta-function potential in the vicinity of the middle of the well but without any abrupt change in the oscillator strength.

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In the last decade, enormous effort has been spent in understanding the physics of quantum well structures because of their applications to electronic and optoelectronic devices.¹ These structures can be fabricated by the molecular beam epitaxy technique, where the thicknesses and fractional molecular constituents of the layers can be controlled precisely and the interfaces sharply defined. The most widely used structure consists of alternate layers of $Al_xGa_{1-x}As$ and $GaAs$ where $Al_xGa_{1-x}As$ has a direct band gap at the Γ -point for Al concentration x less than 0.4. The conduction and valence band differences in $Al_xGa_{1-x}As$ and $GaAs$ layers form the barriers and wells, respectively. A $GaAs$ layer of appropriate thickness sandwiched between the two thick layers of $Al_xGa_{1-x}As$ acts as a quantum well, which has different bound states depending upon the $GaAs$ layer thickness and Al concentration x in the $Al_xGa_{1-x}As$ layers. Recently, transitions between the bound states of the well have received considerable amount of theoretical and experimental attention because of the applicability to photoconductivity² and light absorption.³⁻⁶ It has also been found that with suitably chosen parameters for the quantum well, the structure could be used for infrared detection.⁷⁻¹⁰

Very recently, Trzeciakowski and McCombe¹⁰ performed a theoretical study to tailor the intersubband absorption by considering a thin layer of $Al_yGa_{1-y}As$ in the middle of the well. They found that the presence of a thin barrier in the middle of the well shifts the ground-state energy of the well whereas the first-excited state remains practically unchanged. By changing the concentration y of Al in the middle layer, which determines the height of the barrier, they demonstrated that the energy separation between the ground state and the first-excited state could be changed without appreciably changing the oscil-

lator strength for the ground state to the first-excited state .

In the present Letter, we report the results of an investigation similar to that of Trzeciakowski and McCombe¹⁰ but with a closer look at cases where the height of the middle barrier approaches the energy of the ground state and the first-excited state. A different pattern for the change in the oscillator strength as function of barrier height is found as the barrier height approaches the bound states. It is also found that a similar tailoring can also be achieved by changing the strength of a delta-function potential placed in the vicinity of the middle of the well without any appreciable change in the oscillator strength.

An asymmetric coupled well as shown in Fig. 1 has been considered for investigation. Some approximations such as neglecting the Γ -X mixing when Al concentration y is more than 0.4 and nonparabolicity effects¹¹ which affect the results slightly are made for simplification. We also take a constant effective mass ($0.067m_0$, m_0 being the rest mass of the electron) throughout the structure. The well extends from $-d/2$ to $d/2$ where d is taken to be 150 Å. The thin barrier in the middle extends from $-b/2$ to $b/2$ and three different values of b (5, 10 and 15 Å) are considered in our calculation. For the calculation with delta-function potential in the vicinity of the middle of the well, three different positions ($c = 0, 5, 10$ Å) from the middle of the well are used. All the energies are measured from the bottom of the well. The energies of both the symmetric and antisymmetric bound states are given by the relation

$$\begin{aligned} & \sin^2 \frac{kd}{2} \left[\frac{\bar{K}_L}{k} A_{11} + \frac{\bar{K}_L \bar{K}_R}{k^2} A_{12} + A_{21} + \frac{\bar{K}_R}{k} A_{22} \right] \\ & + \cos^2 \frac{kd}{2} \left[-\frac{\bar{K}_L}{k} A_{11} + A_{12} + \frac{\bar{K}_L \bar{K}_R}{k^2} A_{21} - \frac{\bar{K}_R}{k} A_{22} \right] \end{aligned}$$

$$-\frac{1}{2} \sin kd \left[\left(1 - \frac{\tilde{K}_L \tilde{K}_R}{k^2} \right) A_{11} - \frac{\tilde{K}_L + \tilde{K}_R}{k} A_{12} - \frac{\tilde{K}_L - \tilde{K}_R}{k} A_{21} - \left(1 - \frac{\tilde{K}_L \tilde{K}_R}{k^2} \right) A_{22} \right] = 0. \quad (1)$$

where $k = \sqrt{\frac{2m^*E}{\hbar^2}}$, $\tilde{K}_L = \sqrt{\frac{2m^*(V_L - E)}{\hbar^2}}$, $\tilde{K}_R = \sqrt{\frac{2m^*(V_R - E)}{\hbar^2}}$, m^* is an effective mass, and A is a 2×2 matrix which results from matching the wave functions and their derivatives at the interfaces of the middle barrier or at the delta-function potential. V_L and V_R are the depths of the well as shown in Fig. 1. For the middle barrier extending from $-b/2$ to $b/2$, A is given by

$$A_{11} = \cos kb \cos k_b b + \frac{1}{2} \left(\frac{k_b}{k} + \frac{k}{k_b} \right) \sin kb \sin k_b b. \quad (2a)$$

$$A_{12} = -\sin kb \cos k_b b + \left(\frac{k_b}{k} \cos^2 \frac{kb}{2} - \frac{k}{k_b} \sin^2 \frac{kb}{2} \right) \sin k_b b. \quad (2b)$$

$$A_{21} = \sin kb \cos k_b b + \left(\frac{k_b}{k} \sin^2 \frac{kb}{2} - \frac{k}{k_b} \cos^2 \frac{kb}{2} \right) \sin k_b b. \quad (2c)$$

$$A_{22} = \cos kb \cos k_b b + \frac{1}{2} \left(\frac{k_b}{k} + \frac{k}{k_b} \right) \sin kb \sin k_b b. \quad (2d)$$

when the barrier height V_b is less than E . The same expression can be used when V_b is greater than E by changing k_b to ik_b . Here $k_b = \sqrt{\frac{2m^*(E - V_b)}{\hbar^2}}$. For the delta-function potential located at a distance c from the middle of the well, the matrix A takes the form

$$A = \begin{pmatrix} 1 - \frac{\delta}{2k} \sin 2kc & -\frac{\delta}{k} \cos^2 kc \\ \frac{\delta}{k} \sin^2 kc & 1 + \frac{\delta}{2k} \sin 2kc \end{pmatrix}. \quad (3)$$

where $\delta = \frac{2m^*\delta'}{\hbar^2}$, with δ' as the strength of the delta-function potential measured in $\text{eV} \cdot \text{\AA}$. It is clear from Eqs. (1)-(3) that for the case where V_b or δ' is taken to be zero, A reduces to a unit matrix and Eq. (1) takes the form

$$\frac{\tilde{K}_L + \tilde{K}_R}{k} \cos kd - \left(1 - \frac{\tilde{K}_L \tilde{K}_R}{k^2} \right) \sin kd = 0. \quad (4)$$

which is the condition for the bound states in an asymmetric well of width d . For the symmetric well, since $K_L = K_R \equiv K$, Eq. (4) reduces to

$$\cos kd - \frac{1}{2} \left(\frac{k}{K} + \frac{K}{k} \right) \sin kd = 0, \quad (5)$$

which is the condition for the bound states in a symmetric well of width d .

The oscillator strength for the dipole transition from a state m to a state n is given by

$$f_{mn} = \frac{2m_0(E_n - E_m)}{\hbar^2} | \langle n | x | m \rangle |^2, \quad (6)$$

where m_0 is the rest mass of the electrons, E_n and E_m are the energies of the n and m states, respectively, and $\langle n | x | m \rangle$ is the dipole matrix element.

Equations (1)-(3) can be used to find the symmetric and antisymmetric states of an asymmetric well, and the oscillator strength for the transition between these two states can be calculated by employing Eq. (6). Depending upon the width and depth of the well, if there is more than one excited state then a transition between the symmetric states is forbidden by selection rules. A transition from the ground state to the second-excited state is not allowed, whereas the transition from the first-excited state to the second-excited state is allowed if either of the states is populated by some means.

Figures (2) and (3) show our results for a well of width 150 Å with left and right walls 200 meV and 180 meV deep, respectively, and a thin barrier of width 5, 10 or 15 Å. Panel (a) of Fig. 2 shows the change in the ground-and the first-excited-state energies and the oscillator strength for the transition between them versus the barrier height in the vicinity of the ground state. The insert in the lower half of panel (a) displays the ground state and first-excited wave functions for the barrier height and width of 18 meV and 15

A, respectively. It is quite clear that the oscillator strength remains practically constant for the lower values of V_b . As V_b approaches the ground state, the change brought by the barrier in the ground-state wave function increases the oscillator strength slightly because the barrier remains practically unseen by the excited state, and also the wave function of the excited state vanishes in the vicinity of the middle of the well. The results in panel (b) of Fig. 2 display the changes due to the barrier height in the vicinity of the excited state. In this case the wave function of the ground state goes through a minimum in the barrier region, whereas the wave function of the excited state has an oscillation (due to the formation of an excited state in the small well formed by the excited state and the barrier) in that region, although the wave function still vanishes in the vicinity of the middle of the well (see the insert in the bottom half of panel (b) of Fig. 2). This change in the wave function results in a minimum for the oscillator strength, but the state energies are not affected. In Fig. 3, we show the results when V_b is above the energies of both states. A smooth variation of the oscillator strength as expected is found. The change in the ground-state energy and decrease of the oscillator strength results from the minimum of the ground-state wave function in the barrier region. A similar pattern is also observed for the transition from the first-excited state to the second-excited state but is not shown here in the interest of brevity.

Figure 4 shows the results for a delta-function potential of variable strength placed at 0, 5 or 10 Å away from the middle of the well. The oscillator strength in this case decreases smoothly, even for a small value of the strength of the delta-function potential, because the height of a delta-function potential extends to infinity.

In conclusion, we have carried out a theoretical investigation of the intersubband transitions in an asymmetric quantum well (1) by considering a thin barrier of variable height in the middle of the well or (2) by placing a delta-function potential of variable strength in the vicinity of the middle of the well. In the case of a thin barrier, significant changes in the oscillator strength are noticed as the barrier height approaches the bound state energies, whereas the energies of the states remained unaffected. It has also been found that the tailoring of intersubband transitions is also possible by changing the strength of a delta-function potential placed in the vicinity of the middle of the well without appreciably changing the oscillator strength.

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Figure Captions

- Fig. 1. Schematic diagram of an asymmetric quantum well structure with a thin barrier or a delta-function potential. The parameters taken for the calculation are as follows: $V_L = 200$ meV, $V_R = 180$ meV, $d = 150$ Å, $b = 5, 10$ or 15 Å, and c (position of the delta-function potential away from the middle of the well) = $0, 5$ or 10 Å.
- Fig. 2. Energies of the ground and first-excited states measured from the bottom of the well and their corresponding oscillator strength versus barrier height (i) in the vicinity of the ground state. [panel (a)] and (ii) in the vicinity of the first excited state [panel (b)]. The solid, dashed and dotted curves correspond to barrier widths of $5, 10$ and 15 Å, respectively. The insert in the bottom half of panel (a) displays the ground-state (solid line) and first-excited-state (dotted line) wave functions from -100 to 100 Å spatial dimension for a 18 meV barrier height and 15 Å barrier width. In panel (b) the wave functions are shown for a 64 meV barrier height and 15 Å barrier width.
- Fig. 3. Ground and first-excited-state energies and oscillator strength as in Fig. 2 but for a barrier height above the first-excited state.
- Fig. 4. Energies of the ground and first-excited states measured from the bottom of the well and their corresponding oscillator strengths as a function of the strength of the delta-function potential. The solid,

dashed and dotted curves correspond to $c = 0.5$ and $10 \text{ \AA}$, respectively.

Exactly the same results are found for $c = -5$ and $-10 \text{ \AA}$.

Fig. 1

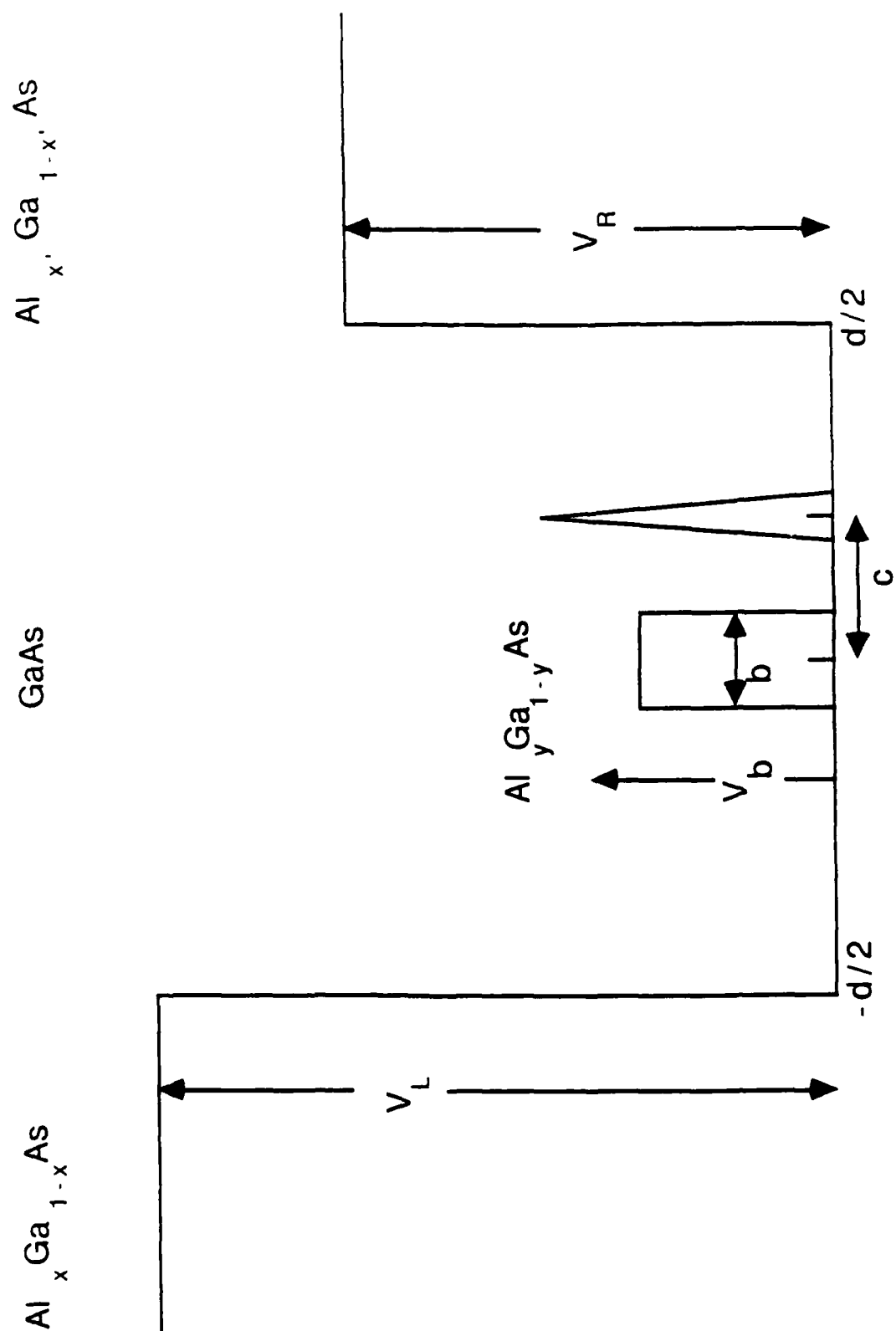


Fig. 2

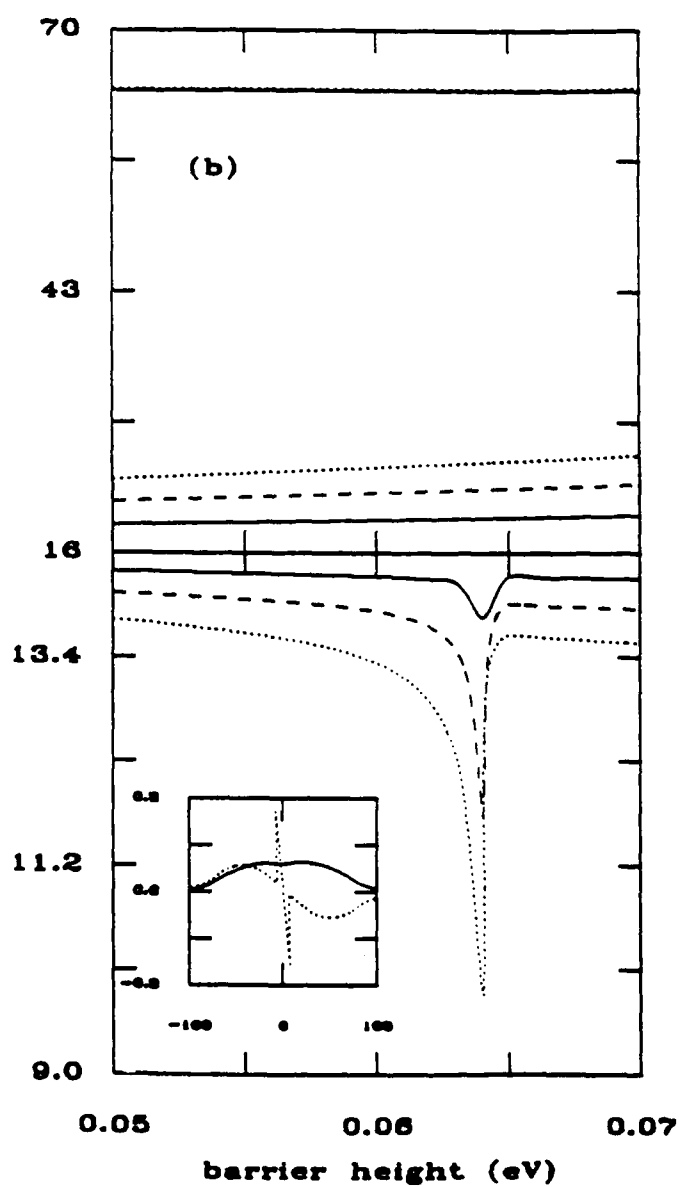
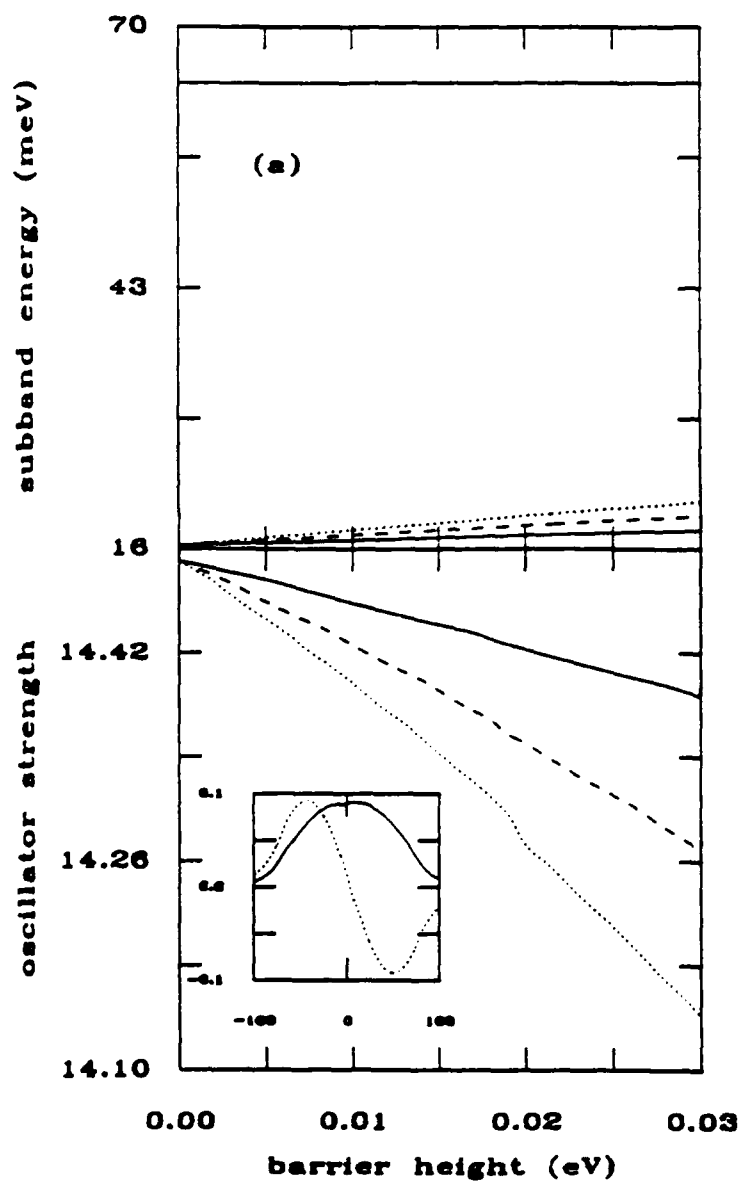


Fig. 3

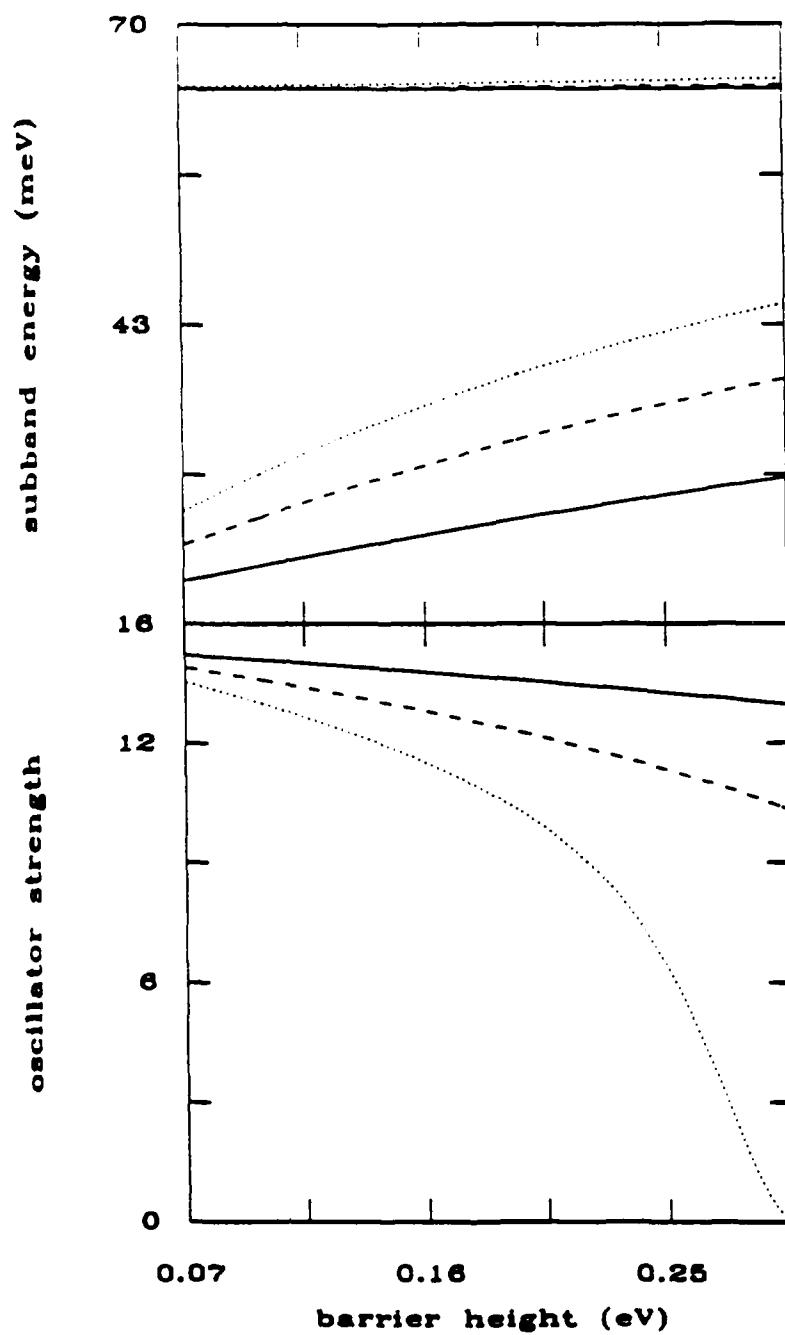
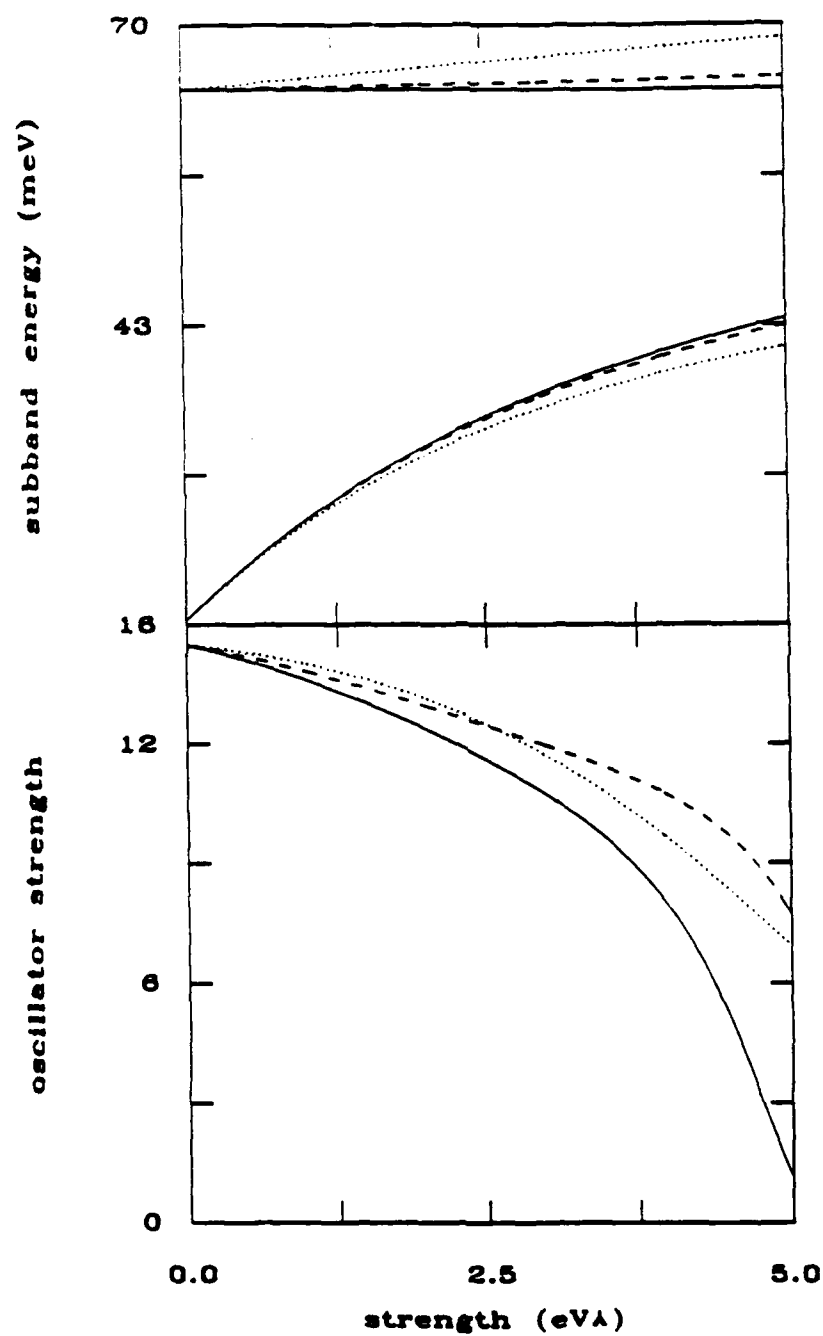


Fig. 4



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