

BAND STRUCTURE OF NON-IDEAL SEMICONDUCTOR SUPERLATTICES

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An ideal superlattice is an array of two (or more) alternating layers of materials with a single period, fixed barrier height and infinitely abrupt interfaces. A real superlattice differs from an ideal one in many aspects and this affects the band structure. They include unsharp interfaces, interface disorder, small fluctuations in thicknesses of quantum wells (barriers) and in the potential barrier heights from layer to layer. The band structure of superlattices in these realistic cases have been investigated. The relevance of these non-ideal cases to the shifting of the ground-state energy of the electrons, holes, and the effective energy gap are also discussed.

The last decade has seen the development of a new semiconductor technology based upon ultrathin structures.[1,2] Molecular beam epitaxy (MBE) has been one of the key epitaxial crystal growth techniques responsible for this new technology. Although it is commonly accepted that MBE is capable of fabricating interfaces between two semiconductors to grow quantum wells (QWs) and superlattices with very high quality, one can never grow superlattices with the ideal structure. Here, an ideal superlattice means an array of two (or more) alternating layers of materials with a single period, fixed well (barrier) width and barrier height, no roughness on the interfaces and infinitely abrupt interfaces. A real superlattice differs from an ideal one in many aspects. They include: (a) Unsharp interfaces,[3] or band bending in the depletion regions; (b) Interface disorder or roughness, or thickness fluctuations within a quantum well (barrier); (c) Fluctuations in the average thickness of the well (barrier) width from layer

to layer; and (d) Fluctuations in the potential barrier height which was caused by the fluctuations of Al concentrations x from layer to layer for GaAs-Al x Ga $_{1-x}$ As superlattices.

As pointed out by us in a previous paper,[3] although advanced techniques such as chemical vapor deposition and molecular-beam epitaxy may produce superlattices with physical interfaces between two materials crystallographically abrupt, the bonding environment of the atoms adjoining this interfaces will change on at least an atomic scale. As the potential form changes from a well (barrier) to a barrier (well), an intermediate potential region exists for the electrons and holes. The effects of interface disorder has been discussed by many groups.[4,5,6] This interface disorder (roughness) caused the linewidth broadening in photoluminescence spectra.[5] It has been mainly shown that when the right growth parameters are obtained, the magnitude of the interface disorder is one atomic monolayer.[7] For the purpose of smoothing the interfaces or enlarging

the lateral size of monolayer growth islands, by interrupting the growth for 2 minutes at each interface, the photoluminescence of the QW sample grew by this method clearly resolved into three peaks which result from the one-monolayer growth islands with the lateral size larger than the exciton diameter.[6] Cases (c) and (d) have never been studied before. In this paper, we will focus on the non-ideal cases (a)-(c), since the main effects caused by the case (d) will be similar to the case(c).

The band profile of the non-ideal superlattice for the cases (a)-(d) has been schematically shown in Fig. 1 where different non-ideal cases have been drawn separately. The real superlattices will be much more complicated in which all the non-ideal cases (a)-(d) will be mixed together.

In Fig. 1(a), we have assumed linear potentials across the interfaces (graded interfaces). At this stage, the exact potential form for the electrons and holes at the interface is unknown. Nevertheless, a linear potential form for the electron and hole across interface is a better approximation compared with infinitely abrupt interfaces. When the interface thickness $\Delta \ll 5 \text{ \AA}$, we can get a simple dispersion relation for the electrons and holes.[3] For simplicity, we consider only the case of small Al concentration ($x < 0.4$), so that the assumption of a simple effective mass of the electron (hole) for the two materials is valid. As an approximation, for the case (a), we have used $m_e = 0.08m_0$ for the average value of the electron effective mass, $m_{hh} = 0.48m_0$ for the heavy holes, and $m_{lh} = 0.09m_0$ for the light holes, where m_0 is the electron mass in free space. In this paper, we focus on the most extensively studied superlattices of GaAs-Ga_{1-x}Al_xAs. The empirical expression, $E_g = 1.155x + 0.37x^2$ eV, for the direct band-gap difference between GaAs and Ga_{1-x}Al_xAs was used.[8,9] The band gap of GaAs is 1.520 eV.[10] The conduction and the valance-band discontinuities at the interface have been suggested to be about 60% and 40%, respectively, of the direct band-gap difference between the two semiconductor materials.[11,12] The unit of energy in this paper is $\hbar^2 \pi^2 / 2m_0 L = 3.76 \text{ meV}$ with $L = 100 \text{ \AA}$.

Fig. 2 is the plot of energy values of electrons (C_1), heavy (HH_1) and light (LH_1) holes at zone-center of the first subband level (ground state) as functions of the period length L with $a=b=L/2$ and $x=0.3$. The dashed

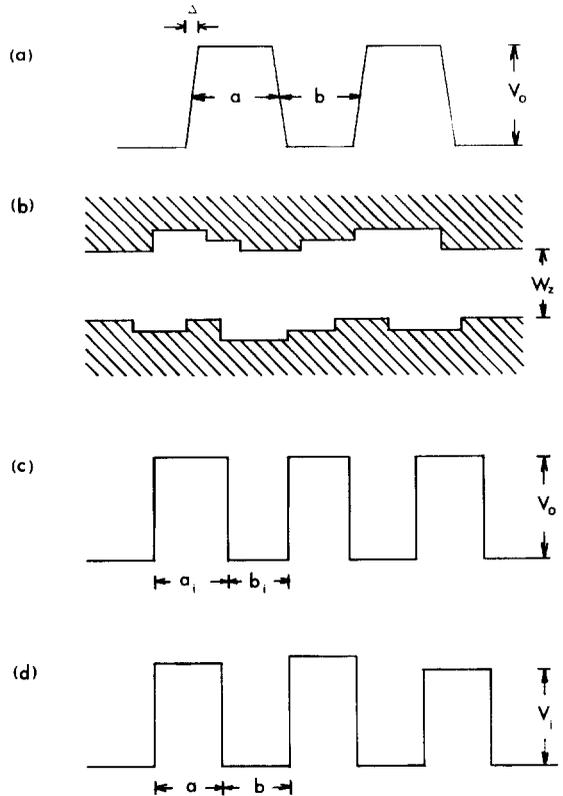


Fig. 1. Band profile of the non-ideal superlattice with (a) Finite widths of the interfaces; (b) Interface disorder; (c) Periodic length disorder; and (d) Al concentration disorder.

and solid lines correspond to the $\Delta = 0$ and $\Delta = 4 \text{ \AA}$, respectively. The effects of this finite interface thickness to the ground-state energies of electrons, heavy and light holes can be obtained from Fig. 2. For the GaAs-Ga_{1-x}Al_xAs superlattice with $x=0.3$ and $a=b=L/2$ at the region $80 \text{ \AA} \leq L \leq 150 \text{ \AA}$, this finite interface thickness $\Delta (=4 \text{ \AA})$ increases all the ground-state energy levels of the electrons and holes. The heavy holes have the largest amount of increase while the light holes have the least amount of increase. The amount of shifts for the ground state of electrons and light holes increase as L increases. The shifts are almost zero at $L=80 \text{ \AA}$ for both electrons and light holes, and increased by about

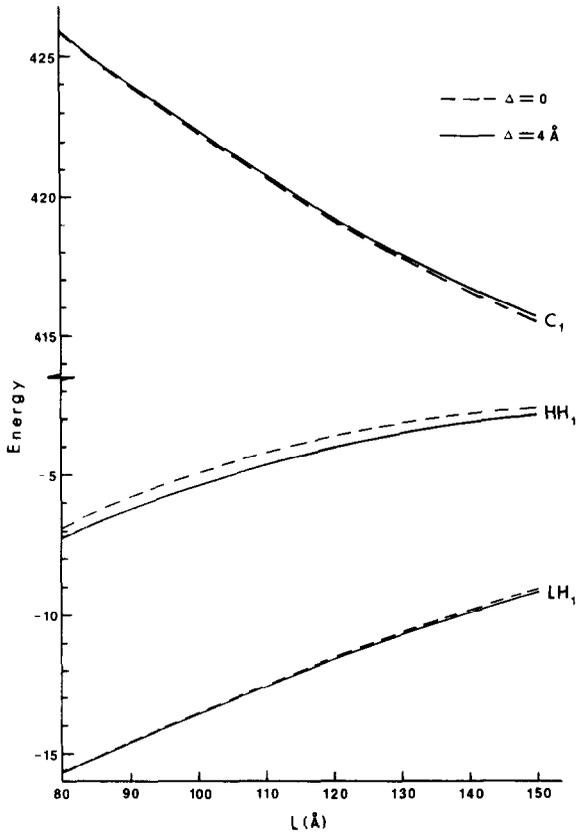


Fig. 2 Ground-state energies of electrons (C_1), heavy (HH_1) and light (LH_1) holes as functions of the period length L with $a=b=L/2$ and $x=0.3$ for $\Delta=0$ (dashed lines) and $\Delta=4 \text{ \AA}$ (solid lines). The unit of energy for all figures is $\frac{\hbar^2 \pi^2}{2m_0 L^2} = 3.76 \text{ meV}$ with $L=100 \text{ \AA}$.

0.15 and 0.07 units for electrons and light holes, respectively at $L=150 \text{ \AA}$. For heavy holes, the amount of shift decreases as L increases from 80 to 150 \AA . From Fig. 2, we can also get the shift of the effective energy-gap for the heavy and light holes as a function of L . Here the effective energy gap represents the minimum energy required for producing excitons. The shift of the effective energy gap are always larger than zero for both heavy and light holes. The amount of shift in effective energy gap is larger for heavy holes than for light holes.[13]

The results in the Fig. 2 can be understood by noting that the shift of

the ground-state energy of electrons and holes can be affected by two factors. One is the position of the energy level inside the potential well and the other one is the interface thickness (Δ) relative to the well width. The ground-state energy of the electrons and holes with a infinitely abrupt interface depend on the period L and they increase as L decrease. For large L , the ground-state energy levels lie close to the bottom of the potential wells. The effective well width, as shown in the Fig. 1(a), decreases at the bottom of the well. This increases the ground-state energy of electrons and holes. The amount of increase depends on the position of the ground-state energy level inside the potential wells. For superlattice with small L , if the energy lie close to the top of the potential well, the ground-state energy will be decreased because of the increase of the effective potential well width. For the heavy holes, the ground-state energy lies more close to the bottom of the potential wells and thus has the largest increase. For the same reason, the ground-state of the light holes lies close to the middle of the potential well and so has the least amount of increase. For the heavy holes, the ground-state energy level lies very close to the bottom of the potential wells, as the well width increases, the enhancement in the energy due to the decrease of the effective well width is not sufficient to counterbalance the reduction due to the ratio of interface thickness to the well width (Δ/a) decreasing. So the total amount of shift decreases as L increases.

Fig. 3 is the plot of $\Delta E_g = E_g(\Delta=4\text{\AA}) - E_g(\Delta=0)$ of heavy ($\Delta E_{g_{hh}}$) and light ($\Delta E_{g_{lh}}$) holes, the shift of the effective energy gap, as a function of Al concentrations x with $L=120 \text{ \AA}$ and $a=b=L/2$. The unit of energy is the same as in Fig. 2. From Fig. 3, we can see that the shift of the effective energy gap for heavy holes monotonically increases as x increases from $x=0+$ (no bound state at $x=0$) to $x=0.35$. For the light holes, $\Delta E_{g_{lh}}$ is negative (~ -0.004) for $x \leq 0.1$, then increases to positive as x increases. The shift of the effective energy gap for heavy holes is always larger than that of the light holes. The difference in $\Delta E_{g_{hh}}$ and $\Delta E_{g_{lh}}$ is also increased as x increases. It means that as x increases, the interface effects is more pronounced for the heavy holes than for the light holes. All these results can be

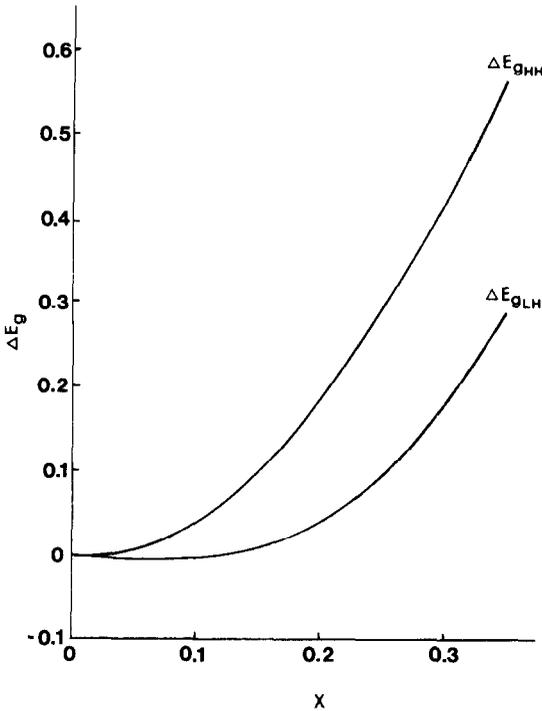


Fig. 3. The shift of the effective energy gap $\Delta E_g = E_g(\Delta = 4A) - E_g(\Delta = 0)$ of heavy (ΔE_{gHH}) and light (ΔE_{gHL}) holes as functions of Al concentrations x with $L=120 \text{ \AA}$ and $a=b=L/2$.

understood by using the same arguments for the results in Fig. 2. For the GaAs-Ga_{1-x}Al_xAs superlattice of $x=0.3$, ΔE_{gHH} is 0.416 (1.56 meV) and ΔE_{gHL} is 0.177 (0.63 meV). We can see that the shifts are quite significant.

The first experiment showing the interfaces disorder came from the observation that the excitation spectrum linewidth increases as the quantum well width decreases.[4,7] It has been explained by the one monolayer fluctuation in the well width. What we want to point out here is that the fluctuation of the one monolayer in the well width is only a necessary condition, but not a sufficient condition, for the linewidth broadening. It is obvious that if the lateral size of the step (islands or domain) is much larger than the Bohr diameter of the exciton, instead of linewidth broadening, one should observe discrete energies corresponding to the different well

size. This has been observed by different groups.[7,14,15] So the important factor for the linewidth broadening comes from the small lateral size step or from the junction between different islands. This contradicts with the prediction of Singh et al.[16] They claimed that the linewidth increases with the island's size. In fact, when the island increases to certain size, the linewidth caused by the interface disorder will go to zero if we neglect the junction effect between different islands. Qualitatively, the linewidth broadening can be understood if we note that the effective well width seen by each exciton depends on the distribution of different lateral size islands within the region of the Bohr diameter of the exciton. Different excitons "see" different effective well thickness, so the effective well width can change continuously in certain regions, corresponding to an energy distribution or linewidth. The small islands (lateral size smaller than the Bohr diameter) are the major effects for the linewidth broadening. At this case, due to randomness, the probabilities that the total areas of islands with well thicknesses of $w_0 + \delta$ and $w_0 - \delta$ for the excitons are the same, therefore we expect an energy shift caused by this interface disorder. Suppose $S(\delta)$ is the distribution function of the total area with well thickness $w_0 + \delta$ and $S(\delta) = S(-\delta)$, when one averages the energy of excitons over the region corresponding to the Bohr diameter of excitons, the increase in energy due to the decrease in well width ($-\delta$) is larger than the decrease in energy due to the increase in well width ($+\delta$). We have, for the exciton energy,

$$E = (1/2X_0) \int_{-X_0}^{X_0} E(w_0 + \delta) S(\delta) d\delta \quad (1)$$

$$= E(w_0) + (1/4X_0) E''(w_0) \int_{-X_0}^{X_0} \delta^2 f(\delta) d\delta$$

where $E(w_0)$ is the energy of excitons within a quantum well with a single width w_0 and X_0 being one or two monolayers depending on the quality of samples. In obtaining Eq.(1), we have used Taylor's expansion and keep the first non-zero term. $E''(w_0)$ is always larger than zero for a quantum well. therefore, we expect a small positive energy shift which is proportional to the second derivative of the energy with respect to the well width w . This shift is due to the small islands within the region of the Bohr diameter of the exciton and is

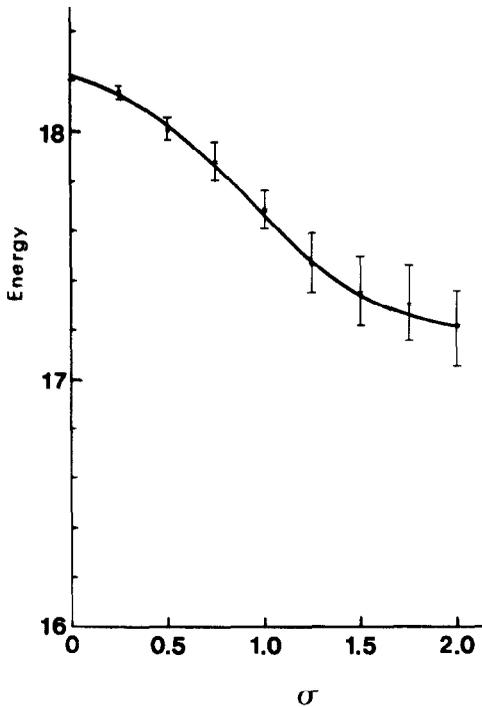


Fig. 4. Ground-state energy (measured from the bottom of the quantum well) of electron as a function of fluctuation parameter σ with $L_0=100$ A, $a_0=b_0=L_0/2$ and $x=0.3$.

completely different than that due to the exciton trapped by the large lateral size islands with a one-monolayer-deeper than average well thickness. It is obvious that the amount of shift depends on the quantum well width and barrier height for the same interface conditions. This shift has been ignored previously for the reason that one believes that the overall effects will canceled each other. The reason one did not notice from experiment is that there are many parameters that can be adjusted to fit the experimental data. In the above discussions, we have ignored the thermalization process which makes excitons favor the larger wells. In fact, when the lateral size step is much smaller than the Bohr diameter of exciton, this can hardly affect the exciton energy.

The periodic length disorder, as shown in Fig. 1(c), is similar to the so called Mott disorder.[17] Fig. 1(d) is corresponding to the so called Anderson disorder.[18] Although we

have familiar potential form here, the physics for the superlattices are completely different from their random one-dimensional potential array. Their system is a disorder system, the most interesting physics is the localized-delocalized transition. For a real superlattice, there is more or less a small fluctuation in well (barrier) thickness, and the most important physics is the effects of this fluctuation to the band structures.

For calculating the band structure, we treat the problem by the following. We allow that the thickness of each well and barrier has a small fluctuation, so that $a_i=a_0+\delta_i^a$ and $b_i=b_0+\delta_i^b$, and so $L_i=L_0+\delta_i$ ($\delta_i=\delta_i^a+\delta_i^b$) is the i th "period length". Because this fluctuation is

random, we should have $\sum_{i=1}^n L_i=nL_0$ for large n , where n represents the total number of "periods" and L_0 is the average "period length". Also we assume that the fluctuation δ_i (δ_i^a and δ_i^b) has the Gaussian distribution:

$$P(\delta_i)=N \exp(-\delta_i^2/2\sigma^2), \tag{2}$$

where N is the normalization constant and σ is the fluctuation parameter. For a real superlattice, there is only a finite number of layers. At the two boundaries, we have the cyclic condition for the wavefunctions of electrons and holes

$$\psi(x=0)=\psi(x=\sum_{i=1}^n L_i).$$

By using the matrix method[19,20] and the continuity conditions of the wavefunction $\psi(x)$ and $(1/m^*)d\psi/dx$ across the interfaces, we can get a dispersion relationship. In this paper, we only calculate the ground-state of electrons and holes with $n=100$.

In the calculation, instead of taking that δ varies continuously, we let δ change by steps. δ has been taken from 0 to +3 A with step of 0.5A and following the distribution of Eq. (2). We averaged ten different groups of random a_i and b_i to calculate the ground-state energy. Fig. 4 is the plot of the ground-state energy of electron (measured from the bottom of the quantum well) as a function of fluctuation parameter σ with $L_0=100$ A, $a_0=b_0=L_0/2$ and $x=0.3$ for the GaAs-Ga_{1-x}Al_xAs superlattices. In the calculation, we have used $M_1=0.067m_0$ for the electron effective mass for GaAs, and $M_2=(0.067+0.093x)m_0$ for the electron effective mass in

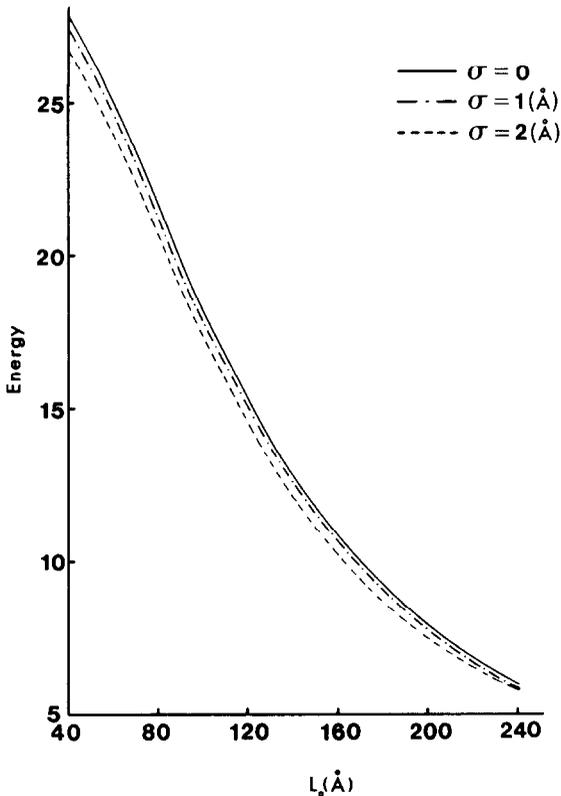


Fig. 5. Ground-state energy of electron (measured from the bottom of the quantum well as a function of L_0 for three different values of fluctuation σ with $a_0 = b_0 = L_0/2$ and $x = 0.3$.

$\text{Ga}_{1-x}\text{Al}_x\text{As}$. All other parameters are the same as mentioned above. From Fig. 4, we can see that the fluctuation can decrease the ground-state energy of electron. The error bars in the figure indicate the standard deviation of the energy from 10 different random sets of a_i and b_i . The physical meaning for this average is that electrons located at different positions "see" different effective well (barrier) width, so the error bars are corresponding to the linewidth broadening caused by this type of disorder in optical experiments. The standard deviation of ground-state energy increases as σ increases, as it should be. The rate of decrease in the ground-state energy is fastest in the region between

$\sigma = 0.5$ to 1.5 Å. As σ increases from 0 (no fluctuation in this case) to 2.0 Å, the total amount of decrease is about 1 unit (3.76 meV). This shift is related to the Mott's mobility edge.[17] It can be understood that the zone-center of the first subband level (ground-state) is mostly determined by the larger "period length" while the zone-edge of the first subband level is more likely to be determined by the smaller "period length". The importance of the result in Fig. 4 is that the ground-state energy can be varied from sample to sample even though the average well and barrier thicknesses are the same. This is probably one of the reasons why different experimental results have been published by different groups. Fig. 4 can also be used to explain why the photoluminescence and absorption lines have blue shift if the incident light intensity increases.[21,22]

Fig. 5 is the plot of ground-state energy of electrons as a function of L_0 for three different fluctuation parameters $\sigma = 0, 1$ and 2 Å with $a_0 = b_0 = L_0/2$ and $x = 0.3$. As we can see from Fig. 5, the fluctuation can increase the ground-state energy for all L_0 and the shift decreases as the L_0 increases. For $L_0 = 40$ Å, the shift between $E(\sigma = 2$ Å), $E(\sigma = 1$ Å) and $E(\sigma = 0)$ are 1.1 and 0.56 units, respectively. So the same fluctuation affects mostly to the small L_0 . In the Fig. 5, we did not indicate the standard deviation of the ground-state energy. It decreases as L_0 increases. This result can be used to explain the experimental observation that linewidth broadening decreases as L_0 increases for the superlattices.

In conclusion, we have investigated the effect to the energy band structure by the non-ideal structures of superlattices. These results can explain some experimental observations. The importance of the investigation for these non-ideal cases is obvious, since they represent the case of the real superlattices. Although some work has been done in this field, many important physical properties, such as electron (hole) mobility, optical emission and absorption, photoluminescence and photoconductivity, perpendicular transport properties affected by the non-ideal structure have never been investigated. Further studies have to be done to understand more physical properties of the real superlattice systems.

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