Superlattice with multiple layers per period

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We have studied the miniband structure of a GaAs-$Ga_{1-x}Al_xAs$ superlattice consisting of double layers of GaAs and $Ga_{1-x}Al_xAs$ materials per period. The variations of widths and gaps of the superlattice minibands are given as functions of the size of the quantum wells in each period; the dependence of the effective energy gap on the size of the quantum wells is also presented.

With recent advances in epitaxial crystal-growth techniques, it has become possible to grow the semiconductor superlattice systems composed of alternate layers of two different semiconductor materials. This leads the band edges to exhibit a periodic variation with the position along the direction of crystal growth. The most extensively studied superlattice is the one consisting of alternate layers of GaAs and $Ga_{1-x}Al_xAs$.[1-7] The GaAs layers form quantum wells and the $Ga_{1-x}Al_xAs$ layers form potential barriers. The energy spectrum of the superlattice can be controlled by the choice of Al concentration in $Ga_{1-x}Al_xAs$, and the thicknesses of the alternate layers. For Al concentration less than about 40% ($x < 0.4$), $Ga_{1-x}Al_xAs$ has a direct band gap at the Γ point.[6] The conduction and the valence-band discontinuity at the interface have been suggested to be about 85% and 15%, respectively, of the direct band-gap difference between the two semiconductors.[2,3,5,7]

Esaki, Chang, and Mendez[8] recently proposed the idea of polytype (ABC) superlattices and applied it to the case of InAs-GaSb-AlSb multiheterojunctions. Bastard[9] also discussed the dispersion relation of polytype superlattices by using the envelope-function approximation. Compared with binary (AB) superlattices, a polytype superlattice provides additional degrees of freedom. On the other hand, it has more complex properties which introduce additional difficulties in fabrication and in physical treatments. In this paper, we have investigated the band structure of a binary GaAs-$Ga_{1-x}Al_xAs$ superlattice consisting of double layers of GaAs and $Ga_{1-x}Al_xAs$ materials per period. The band structure in terms of the potential-barrier height (or equivalently, the x value) and the sizes of the quantum wells and barriers in each period have been calculated. Experimentally, no additional difficulties will be encountered in growing the superlattice of this type compared with those in the growth of the usual lattices (one well and one barrier in each period). The unusual band structure arising from this periodic structure will be useful in technological applications. For the usual superlattices, only three variables (thicknesses of the well and barrier layers in each period, and the height of the potential barrier) are used. If additional layers are introduced in each period, more parameters will be available for getting the desired electronic, optical, and other physical properties.

The compositional semiconductor superlattice, as shown in Fig. 1, is a periodic sequence of ultrathin layers of two different semiconductors. In Fig. 1, b_1 (b_2) denotes the thickness of the first (second) layer of the well material in each period and L the periodic length. The periodic potential barriers are assumed in the analysis to be infinitely repeated. The calculation of the miniband structure was based on the assumptions that the mean free path of the electron (hole) is much larger than the superlattice period, so the collision effects may be neglected; and that the interfaces between the layers are sharply defined so as to be devoid of any surface effect, so the superlattice potential distribution may simply be considered as an one-dimensional array of rectangular wells. In addition, different values for the effective mass in both the barrier and the well materials have been used. Using the matrix method[10] and the continuity conditions of the wave function $\psi(x)$ and $(1/m^*)\partial\psi/\partial x$ across the interface, we obtain the dispersion relation

$$\cos(qL) = (\alpha_1\alpha_2 - \beta_1\beta_2)\cos(kL) + \gamma_1\gamma_2\cos[k(b_1 - b_2)] + (\alpha_1\beta_2 + \alpha_2\beta_1)\sin(kL) \ , \quad (1)$$

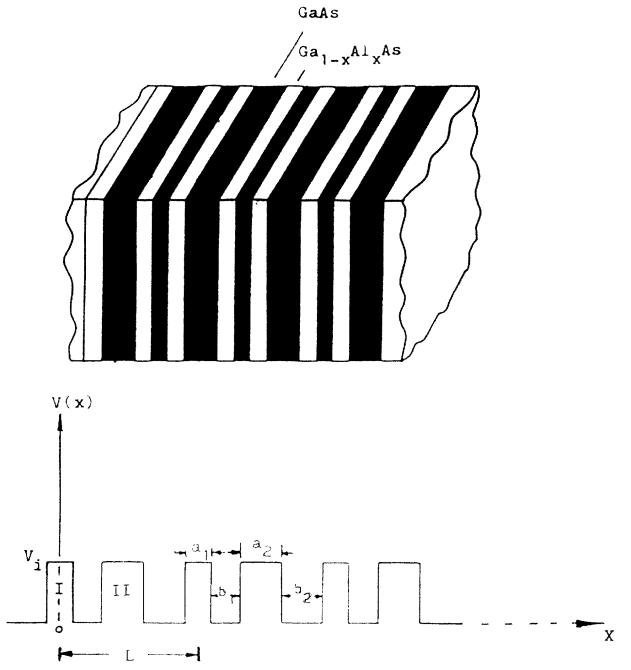

FIG. 1. Schematic superlattice. (a) Compositional superlattice consisting of double layers of GaAs and $Al_xGa_{1-x}As$ materials per period. (b) Band profile of the superlattice showing the periodic potential arising from the band-gap difference between GaAs and $Al_xGa_{1-x}As$.

where

$$\alpha_i = \cos(ka_i)\cosh(Ka_i) - (\epsilon/2)\sinh(Ka_i)\sin(ka_i) \ ,$$

$$\beta_i = \sin(ka_i)\cosh(Ka_i) + (\epsilon/2)\sin(Ka_i)\cos(ka_i) \ , \qquad (2)$$

$$\gamma_i = (\eta/2)\sinh(Ka_i) \ ,$$

and

$$\epsilon = Km_1/km_2 - km_2/Km_1 \ , \quad \eta = Km_1/km_2 + km_2/Km_1 \ , \qquad (3)$$

$$K = [2m_2(V_i - E)]^{1/2}/\hbar \ , \quad k = (2m_1E)^{1/2}/\hbar \ .$$

In Eq. (3), E is the energy of the electron (hole); m_1 and m_2 are, respectively, the effective masses in the well and the barrier materials, and $V_i = V_e$ (or V_h). The method used here may easily be applied to solve for the miniband structure of the superlattice consisting of many layers per period.

In our calculations, we have used $m_1 = 0.067m_e$ for the electron effective mass for GaAs, $m_2 = (0.067 + 0.083x)m_e$ for the electron effective mass in $Ga_{1-x}Al_xAs$, and the empirical expression $E_g = 1.155x + 0.37x^2$ eV for the direct band-gap difference between GaAs and $Ga_{1-x}Al_xAs$.[5-7]

Figure 2 presents the variations of widths and gaps of the conduction minibands as functions of Z $(= b_2/b_1)$, the size ratio of the quantum wells in each period, for particular choices of $x = 0.3$ ($V_e = 0.3228$ eV), period $L = 150$ Å, and barrier widths $a_1 = a_2 = 15$ Å. We see that the width of the lowest-energy miniband increases if Z increases and is a maximum at $Z = 1$ $(b_1 = b_2)$. One should recognize that at $Z = 1$, our potential becomes a Kronig-Penney model of period length of $L' = L/2$. The position of the first minigap for our potential appears at $k = \pi/L$ or $k = \pi/2L'$. In contrast with the result that the first minigap for the Kronig-Penney model is at $k = \pi/L'$, the value $k = \pi/2L'$ corresponds to an energy value within the lowest miniband when $Z = 1$. We see that as Z approaches 1, the lowest and the second conduction minibands become continuous and the first minigap at $k = \pi/L$ reduces to zero. The same results also exist for higher odd minigaps. Figure 2 also shows that there exists a particular choice of Z for which the second and the third minibands yield a continuous band and the second minigap at $k = 2\pi/L$ is zero. By inspection of Fig. 2, we see that, for a fixed choice of compositional material, by changing the layer thicknesses of the wells (barriers) in each period, the energy spectrum of the superlattice can vary over a wide limit.

Figure 3 are the plots of the energy gap between the lowest conduction miniband and the uppermost valence miniband (effective energy gap) versus Z. Neglecting the Coulomb and phonon interactions, the effective gap represents the minimum energy required for producing excitons. Using the Al concentration $x = 0.3$, we get[11-14] $V_e = 0.3228$ eV and $V_h = 0.057$ eV, $m_1 = 0.45m_e$ and

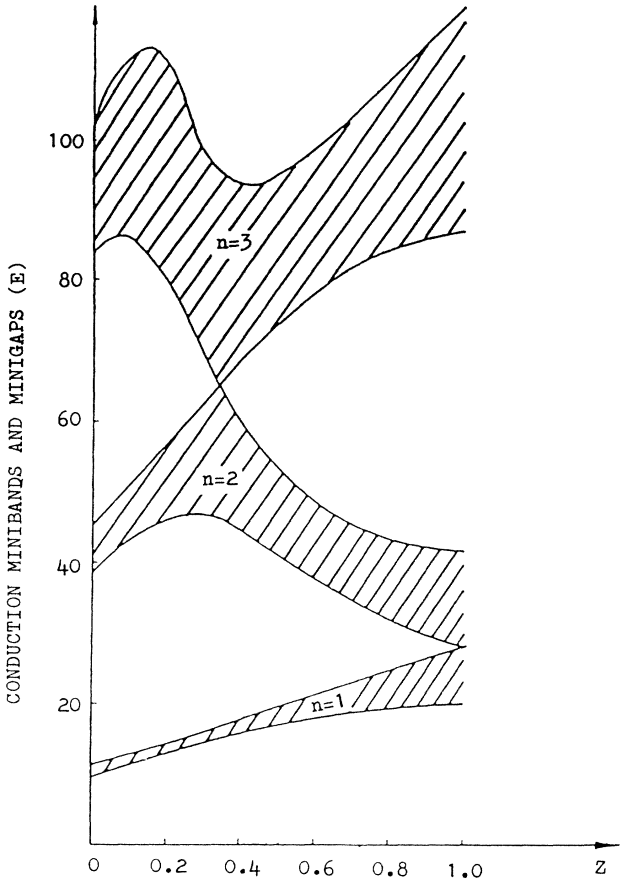

FIG. 2. The first three allowed conduction minibands (shaded area) and minigaps as functions of $Z(= b_2/b_1)$ for $L = 150$ Å, $a_1 = a_2 = 15$ Å, and $x = 0.3$. The energy unit E is $\hbar\pi^2/2m_eL^2$ (1.67 meV).

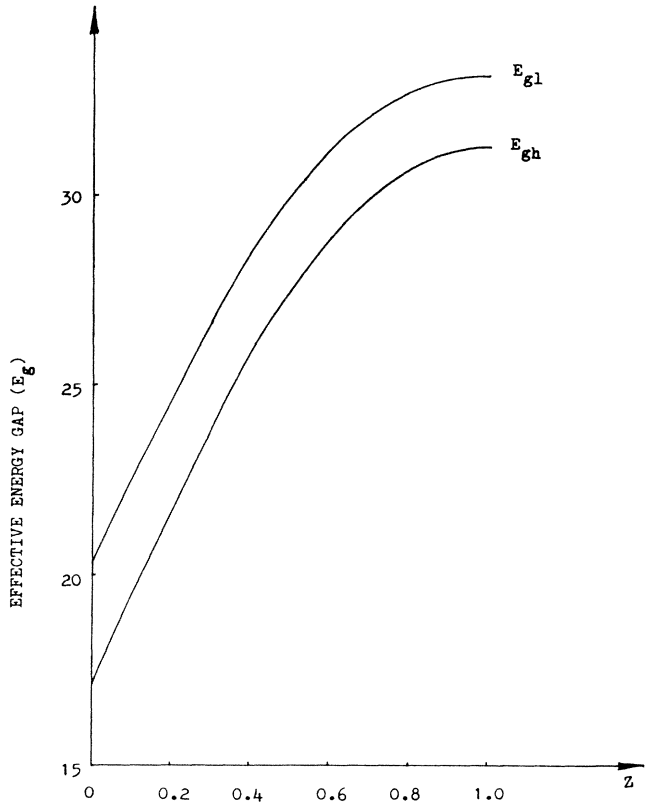

FIG. 3. Effective energy gap vs Z for both heavy (E_{gh}) and light (E_{gl}) holes. All parameters are the same as used in Fig. 2.

$m_2 = 0.51 m_e$ for the heavy holes, and $m_1 = 0.08 m_e$ and $m_2 = 0.102 m_e$ for the light holes.

Figure 3 shows that, in the region of $Z < 0.5$, the effective energy gap for both heavy and light holes increases linearly as Z increases, and is a maximum at $Z = 1$. We also noticed that the absolute energy values of the lowest conduction miniband and the uppermost valence miniband increase as Z increases. For a fixed choice of compositional material, depending on the "design" of the superlattice, the effective energy gap may vary arbitrarily over a wide range.

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