Electronic structures of $Ga_{1-x}In_xN_yAs_{1-y}$/GaAs compressively strained quantum wells

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In recent years, a novel compound semiconductor alloy, GaInNAs, has received considerable attention owing to the growing interest in its fundamental physics and device applications in high performance laser diodes emitting at 1.3 um optical fiber window, and high efficiency multi-junction solar cells. The 1.3 um room temperature CW operation of $Ga_{0.7}In_{0.3}N_{0.01}As_{0.99}$/GaAs compressively strained QW laser has been reported. In order to understand the band structure, optical properties and optimal laser configuration, the electronic structures of the $Ga_{1-x}In_xN_yAs_{1-y}$/GaAs compressively strained quantum wells are investigated using 6×6 Hamiltonian model including the heavy hole, light hole and spin-orbit splitting band.

$$H_v = \begin{bmatrix} H+V(z) & \boldsymbol{a} & \boldsymbol{b} & 0 & i\boldsymbol{a}/\sqrt{2} & -i\sqrt{2}\boldsymbol{b} \\ \boldsymbol{a}^* & L+V(z) & 0 & \boldsymbol{b} & i[\sqrt{2}\boldsymbol{e}-\frac{D}{\sqrt{2}}] & i\sqrt{3/2}\boldsymbol{a} \\ \boldsymbol{b}^* & 0 & L+V(z) & -\boldsymbol{a} & -i\sqrt{3/2}\boldsymbol{a}^* & i[\sqrt{2}\boldsymbol{e}-\frac{D}{\sqrt{2}}] \\ 0 & \boldsymbol{b}^* & -\boldsymbol{a}^* & H+V(z) & -i\sqrt{2}\boldsymbol{b}^* & -i\boldsymbol{a}^*/\sqrt{2} \\ -i\boldsymbol{a}^*/\sqrt{2} & i[\frac{D}{\sqrt{2}}-\sqrt{2}\boldsymbol{e}] & i\sqrt{3/2}\boldsymbol{a} & i\sqrt{2}\boldsymbol{b} & S+V(z) & 0 \\ i\sqrt{2}\boldsymbol{b}^* & -i\sqrt{3/2}\boldsymbol{a}^* & i[\frac{D}{\sqrt{2}}-\sqrt{2}\boldsymbol{e}] & i\boldsymbol{a}/\sqrt{2} & 0 & S+V(z) \end{bmatrix}$$

$$H = \frac{\hbar^2}{2m_0}[(k_x^2+k_y^2)(g_1+g_2)+k_z^2(g_1-2g_2)]-e(z),$$

$$L = \frac{\hbar^2}{2m_0}[(k_x^2+k_y^2)(g_1-g_2)+k_z^2(g_1+2g_2)]+e(z),$$

$$a = \frac{\hbar^2}{2m_0}2\sqrt{3}[k_z(ik_y-k_x)g_3],$$

$$b = \frac{\hbar^2}{2m_0}\sqrt{3}[2ik_xk_yg_3-(k_x^2-k_y^2)g_2],$$

$$D = \frac{\hbar^2}{2m_0}[2(k_x^2+k_y^2)g_2-4k_z^2g_2],$$

$$S = \frac{\hbar^2}{2m_0}[(k_x^2+k_y^2+k_z^2)g_1]+\Delta_0,$$

$$e(z) = \begin{cases} b(1+2c_{12}/c_{11})e_{xx}, & in\ well\ . \\ 0, & in\ barrier\ . \end{cases}$$

$$V(z) = \begin{cases} V_0\ , & in\ barrier\ . \\ 0\ , & in\ well\ . \end{cases}$$

$V(z)$ is the periodic potential of MQWs, b is the valence-band deformation potential, Δ_0 is the spin-orbit split-off energy, m_0 is the free-electron mass, and $\gamma_1, \gamma_2, \gamma_3$ are the Luttinger parameters.

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The in-plane strain e_{xx} is equal to $(a_s-a_0)/a_0$, where a_s is the unstrained lattice constant of $Ga_{1-x}In_xN_yAs_{1-y}$ and a_0 the lattice constant of GaAs. The c_{11} and c_{12} are the elastic stiffness constants.

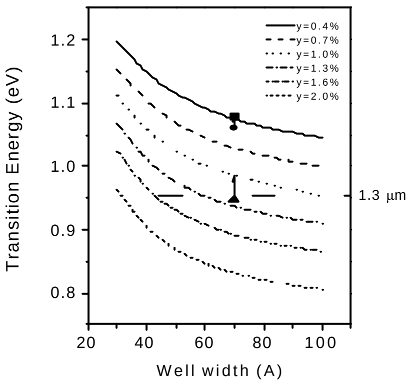

Fig. 1. Ground state transition energies for the $Ga_{1-x}In_xN_yAs_{1-y}$/GaAs MQWs.

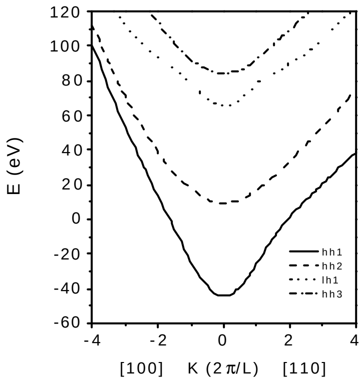

Fig. 2. The energy dispersion for valence band of ww=60Å, y=1.3% $Ga_{1-x}In_xN_yAs_{1-y}$/GaAs MQW.

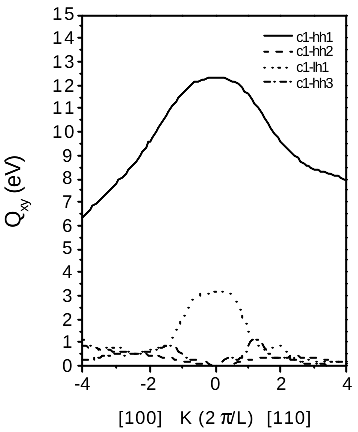

Fig. 3. The squared optical transition matrix elements for TE mode of ww=60Å, y=1.3% $Ga_{1-x}In_xN_yAs_{1-y}$/GaAs MQW.

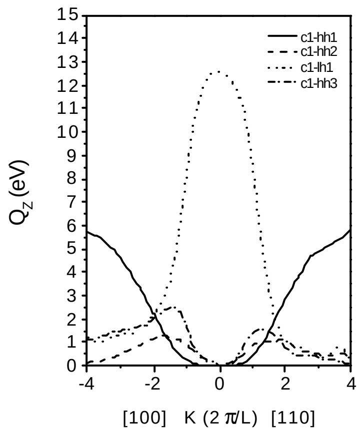

Fig. 4. The squared optical transition matrix elements for TM mode of ww=60Å, y=1.3% $Ga_{1-x}In_xN_yAs_{1-y}$/GaAs MQW.

By varying the well width(ww) and mole fraction(y) of N in the well material, the effects of quantum confinement and compressive strain are examined. The curves of dependence of ground state transition energy on well width and N mole fraction are given in Fig. 1. The square is Chow et al's calculation result for ww=70Å and y=0.4%.The dot is Kondow et al's experimental result for ww=70Å and y=0.4%. The triangle is Kitatani et al's experimental result for ww=70Å and y=1%. The in-plane dispersion curves of hole subbands of $Ga_{1-x}In_xN_yAs_{1-y}$/GaAs MQW are shown in Fig. 2. The first four energy states are identified as hh1, hh2, lh1, and hh3 in our calculation. The TE and TM squared optical transition matrix elements for ww=60Å and y=1.3% for emitting 1.3 um wavelength are given in Fig. 3 and Fig. 4, respectively. The transitions from the valence bands to conductions bands obey the selection rule $\Delta n=0$ at the k=0 point. At the $k\neq0$ points, the $\Delta n=0$ selection rule does not hold. There is band mixing between heavy hole and light hole. The spin-orbit split-off hole mixing can be neglected due to the larger spin-orbit split-off energy Δ_0.