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Calculation of Valence Subband Structures for Strained Quantum-Wells by Plane Wave Expansion Method Within 6×6 Luttinger-Kohn Model*

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Abstract: The valence subband energies and wave functions of a tensile strained quantum well are calculated by the plane wave expansion method within the 6×6 Luttinger-Kohn model. The effect of the number and period of plane-waves used for expansion on the stability of energy eigenvalues is examined. For practical calculation, it should choose the period large sufficiently to ensure the envelope functions vanish at the boundary and the number of plane waves large enough to ensure the energy eigenvalues keep unchanged within a prescribed range.

Key words: semiconductor optical amplifier; strained quantum well; plane wave expansion method; polarization
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1 Introduction

Strained semiconductor quantum-wells have been extensively analyzed because of their abilities to improve the performance of quantum well optoelectronic devices and to realize polarization insensitive semiconductor optical amplifiers. In the analysis, a 6×6 Hamiltonian from the theory of Luttinger-Kohn and Bir-Pikus[1], which describes the strain-caused coupling of the heavy-hole, light-hole, and spin-orbit split-off (SO) bands, is usually employed. An effective-mass equation based on the 6×6 Hamiltonian[1] can be solved to obtain the subband energies and wave functions. Several methods such as the transfer matrix method[2] and the finite difference method[3], etc. have been introduced to solve this equation. The transfer matrix method is very effective for the 4×4 Hamiltonian case[1], i. e., only considering the coupling of the heavy-hole and light-hole bands. However, it becomes very complicated if considering the 6×6 Hamiltonian case, so it is seldom used in this case. The finite difference method is straitforward and easy to implement, but it needs to solve eigenvalues and eigenvectors of very large dimensional matrixes. This involves great computation effort and is difficult to implement on a personal computer.

In this paper, we solve the effective-mass equation by using the plane wave expansion method[4], which can be easily implemented just as the finite difference method but needs much less computation effort. Expanding the envelope function by orthogonal and normalized plane waves, we can transfer the Hamiltonian into a matrix of moderate dimensions. The subband energies and wave

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functions with prescribed accuracy can be efficiently calculated by solving the eigenvalues and eigenvectors of the resulted Hamiltonian matrix.

2 Plane wave expansion method

For a strained semiconductor quantum well grown on the (001)-oriented InP substrate with biaxial-strain, the strain tensor is defined as:

$$\epsilon_{xx} = \epsilon_{yy} = \frac{a_0 - a}{a},$$
$$\epsilon_{zz} = -\frac{2C_{12}}{C_{11}}\epsilon_{xx} \tag{1}$$

where a_0 and a represent lattice constants of the substrate and the quantum well, respectively; C_{11} and C_{12} represent stiffness constants. Under the axial approximation[2], the 6×6 Hamiltonian can be simplified into a block-diagonal form[2,3]:

$$H = \begin{bmatrix} H^{U}_{3\times3} & 0 \\ 0 & H^{L}_{3\times3} \end{bmatrix},$$

$$H^{\sigma}_{3\times3} = -\begin{vmatrix} P+Q-V_h(z) & -R_\rho \mp \mathrm{i}S_\rho & -\sqrt{2}R_\rho \pm \frac{\mathrm{i}}{\sqrt{2}}S_\rho \\ -R_\rho \pm \mathrm{i}S_\rho & P-Q-V_h(z) & \sqrt{2}Q \pm \mathrm{i}\sqrt{\frac{3}{2}}S_\rho \\ -\sqrt{2}R_\rho \mp \frac{\mathrm{i}}{\sqrt{2}}S_\rho & \sqrt{2}Q \mp \mathrm{i}\sqrt{\frac{3}{2}}S_\rho & P+\Delta(z)-V_h(z) \end{vmatrix} \begin{matrix} |U_1^\sigma\rangle \\ |U_2^\sigma\rangle \\ |U_3^\sigma\rangle \end{matrix} \tag{2}$$

where σ is for U or L, which decides the choice of sign of plus or minus in the above matrix, and

$$\begin{aligned} &P = P_k + P_\epsilon, Q = Q_k + Q_\epsilon, \\ &P_k = \left(\frac{\hbar^2}{2m_0}\right)\gamma_1(k_\rho^2 + k_z^2), Q_k = \left(\frac{\hbar^2}{2m_0}\right)\gamma_2(k_\rho^2 - 2k_z^2), \\ &P_\epsilon = -a_v(\epsilon_{xx}+\epsilon_{yy}+\epsilon_{zz}), Q_\epsilon = -\frac{b}{2}(\epsilon_{xx}+\epsilon_{yy}-2\epsilon_{zz}), \\ &R_\rho = -\left(\frac{\hbar^2}{2m_0}\right)\sqrt{3}\left(\frac{\gamma_2+\gamma_3}{2}\right)k_\rho^2, \\ &S_\rho = \left(\frac{\hbar^2}{2m_0}\right)2\sqrt{3}\gamma_3 k_\rho k_z, \\ &k_\rho = \sqrt{k_x^2 + k_y^2} \end{aligned} \tag{3}$$

where k_x and k_y represent plane-wavevectors; k_z is interpreted as a differential operator $-\partial/\partial z$; γ_1, γ_2 and γ_3 represent Luttinger parameters; a_v and b represent Bir-Pikus deformation potentials; $\Delta(z)$ represents the spin-orbit split-off energy; $V_h(z)$ represents the unstrained valence band edge. Here the energy zero is taken to be top of the unstrained valence band edge (i.e. $V_h(z)=0$) in the well region. $|U_1^\sigma\rangle$, $|U_2^\sigma\rangle$ and $|U_3^\sigma\rangle$ are the new basis set corresponding to heavy hole, light hole, and split-off bands, respectively. Their detailed relations with the original basis set i.e. Bloch wave functions $|3/2, \pm3/2\rangle$, $|3/2, \pm1/2\rangle$ and $|1/2, \pm1/2\rangle$ can be found in Reference[2]. The simplified effective-mass equation can be written as

$$\sum_{v=1}^{3} H^{\sigma}_{3\times3,\mu v} g_v^{m,\sigma}(k_\rho, z) = E^{m,\sigma}(k_\rho) g_\mu^{m,\sigma}(k_\rho, z) \tag{4}$$

where m refers to the number of subband, $g_v^{m,\sigma}(k_\rho, z)$ represents the envelope function, and $E^{m,\sigma}$ represents the subband energy.

To ensure the Hamiltonian in Eq. (4) to be Hermitian, all of the operators of forms $A(z)k_z^2$ and $B(z)k_z$ should be replaced with $k_zA(z)k_z$ and $(B(z)k_z + k_zB(z))/2$[3]. We put the quantum well into an assumed large box with the well located at the center. The boundary conditions at the walls of the box will not affect much if we just consider confined states. The side length of the box is so large that the envelope functions vanish at the walls. For convenience, a periodic boundary condi-

tion is imposed so that orthogonal and normalized plane waves can be introduced and the envelope functions can be expanded as

$$g_v^{m,\sigma}(k_\rho, z) = \sum_{p=-\infty}^{\infty} a_{v,p}^{m,\sigma}(k_\rho)|p\rangle,$$
$$|p\rangle = \exp(i2p\pi z/l)/\sqrt{l} \tag{5}$$

where p represents an integer and l represents the period. Substituting Eq. (5) into Eq. (4), we get

$$\sum_{v=1}^{3} H_{3\times3,\mu v}^{\sigma}\Big(\sum_{p=-\infty}^{\infty} a_{v,p}^{m,\sigma}(k_\rho)|p\rangle\Big) = E^{m,\sigma}(k_\rho)\Big(\sum_{p=-\infty}^{\infty} a_{\mu,p}^{m,\sigma}(k_\rho)|p\rangle\Big) \tag{6}$$

Left-multiplying Eq. (6) with the plane wave $\langle q|$, we transform the equation into a matrix form

$$\sum_{v=1}^{3}\sum_{p=-\infty}^{\infty}\langle q|H_{3\times3,\mu v}^{\sigma}|p\rangle a_{v,p}^{m,\sigma}(k_\rho) = E^{m,\sigma}(k_\rho)a_{\mu,q}^{m,\sigma} \tag{7}$$

$H_{3\times3,\mu v}^{\sigma}$ can be expressed as the sum of several generalized items such as $k_z A(z) k_z$ and $(B(z)k_z + k_z B(z))/2$ and $C(z)$, where $A(z)$, $B(z)$ and $C(z)$ are step functions of z, i.e. they have different values for the well and barrier region, which are indicated by the subscript w and b, respectively. Taking the center of the well at $z = 0$, we can calculate $\langle q|H_{\mu v}^{\sigma}|p\rangle$ based on

$$\left.\begin{aligned}
\langle q|k_z A(z) k_z|p\rangle &= \Big(\frac{2\pi}{l}\Big)^2 pq\Big[A_b + (A_w - A_b)\frac{\sin[(p-q+\xi)\pi\frac{d_w}{l}]}{\pi(p-q+\xi)}\Big]\\
\langle q|(k_z B(z) + B(z)k_z)/2|p\rangle &= \frac{2\pi}{l}\times\frac{p+q}{2}\Big[B_b + (B_w - B_b)\frac{\sin[(p-q+\xi)\pi\frac{d_w}{l}]}{\pi(p-q+\xi)}\Big]\\
\langle q|C(z)|p\rangle &= C_b + (C_w - C_b)\frac{\sin[(p-q+\xi)\pi\frac{d_w}{l}]}{\pi(p-q+\xi)}
\end{aligned}\right\} \tag{8}$$

where d_w and d_b represent the widths of the well and barrier, respectively, the period $l = d_w + d_b$, and ξ represents an infinitesimal. In practical calculation, we use a finite number of plane-waves as an approximation to implement the expansion. If p varies from $-N$ to N, i.e. and $2N+1$ plane-waves are used, the Hamiltonian becomes a $6N+3$ dimensional matrix. Through solving its eigenvalues and eigenvectors we can obtain the valence subband energies and wave functions.

3 Numerical results

We considered a quantum well structure with a 6nm $In_{0.4}Ga_{0.6}As$ (tensile strain) well and InP barriers. The parameters listed in paper[2] were used in the following calculation. For the conduction-band and valence-band offsets, $\Delta E_c = 0.36\Delta E_g$ and $\Delta E_v = 0.64\Delta E_g$ were assumed. The first several subband energy dispersions were shown in Fig. 1, in which the data were obtained under the condition that 61 plane-waves used for the expansion and the period l equal to 20nm. It can be seen that the first subband becomes a light hole subband because of the tensile strained quantum well structure. The envelope functions for the LH1 subband

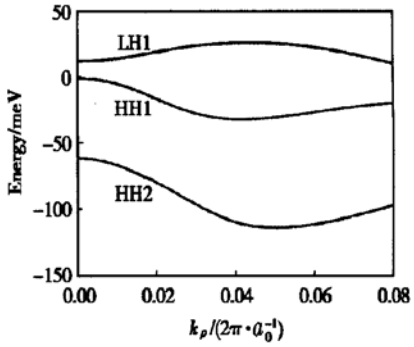

Fig. 1　Energy dispersions for the first three subbands of the tensile strained $In_{0.4}Ga_{0.6}As$-InP quantum well with the well width 6nm

at $k_\rho = 0.02\times2\pi/a_0$ were shown in Fig. 2. It is clear that the second component $g_2^{1,u}$ i.e. the light hole component is much larger than the other two components, so it is denoted as a light hole subband. But for the HH1 subband, it is so different that the first heavy hole component is much larger than

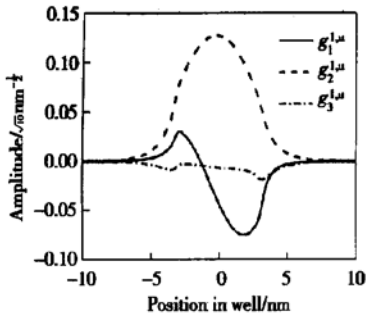

Fig. 2 Envelope wave functions for the LH1 subband of the tensile strained $In_{0.4}Ga_{0.6}As$-InP quantum well with the well width of 6nm and $k_\rho = 0.02\times 2\pi/a_0$

others as shown in Fig. 3. For certain period l, the number of plane waves used for expansion should be large enough to ensure the eigenvalues unchanged in a prescribed range. In Fig. 4 we plotted the energy eigenvalue of the LH1 subband at $k_\rho = 0.02\times 2\pi/a_0$ versus the number of plane waves

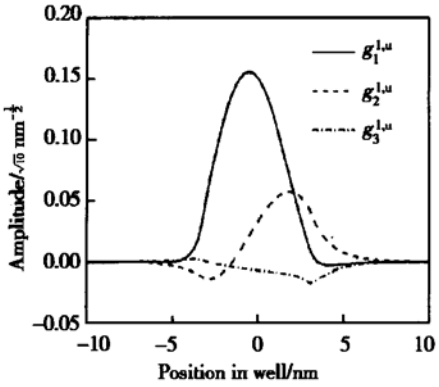

Fig. 3 Envelope wave functions for the HH1 subband of the tensile strained $In_{0.4}Ga_{0.6}As$-InP quantum well with the well width of 6nm and $k_\rho = 0.02\times 2\pi/a_0$

$2N+1$ used for expansion. The period l was set to be 20nm and N varied from 10 to 60. It can be seen that the energy eigenvalue keeps unchanged within a range of 0.1meV for N larger than 30. As to the period l, it should be chosen large enough to ensure the envelope functions vanish at the boundary. In Fig. 5, we showed the energy eigenvalue versus the period l, the number of plane waves were chosen to keep the eigenvalues unchanged within a range of

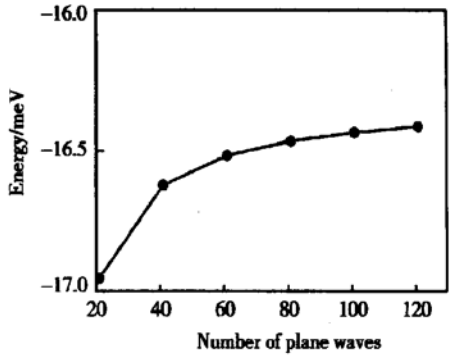

Fig. 4 Energy eigenvalue of the LH1 subband at $k_\rho = 0.02\times 2\pi/a_0$ versus the number plane-waves used for expansion

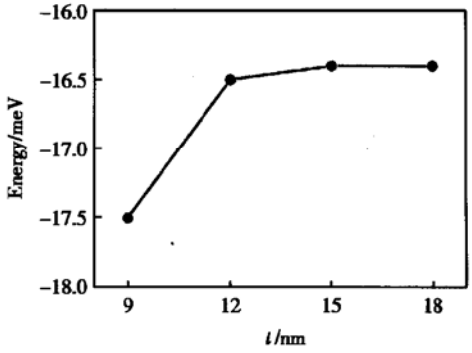

Fig. 5 Energy eigenvalue of the LH1 subband at $k_\rho = 0.02\times 2\pi/a_0$ versus the period l

0.1meV. We can see that the eigenvalues keeps unchanged for l that is larger than 15nm, but for larger periods more plane waves are needed for expansion, which means more computation effort. In practical calculation, we should choose suitable l and N to ensure required accuracy and save time of computation simultaneously.

4 Conclusion

We have used the plane-wave expansion method in calculating the valence subband energies and wave functions for a tensile-strained quantum well within the 6×6 Luttinger-Kohn model. We have also introduced the principles to select the period and number of the plane waves used for the expansion to obtain the required accuracy. The obtained subband energies and wave functions form

the basis of further calculation of the gain for strained quantum wells and the design for polarization insensitive semiconductor optical amplifiers.

References

[1] Chuang S L. Physics of optoelectronic devices. New York: Wiley, 1995

[2] Chao C Y P, Chuang S L. Phys Rev B, 1992, 46: 4110

[3] Chang C S, Chuang S L. IEEE J Select Topics Quantum Electron, 1995, 1: 218

[4] Li Shushen, Xia Jianbai. Acta Physica Sinica (overseas edition), 1997, 6: 848

用 6×6 Luttinger-Kohn 模型和平面波展开方法计算应变量子阱材料的价带结构*

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摘要：用 6×6 Luttinger-Kohn 模型结合平面波展开方法计算了应变量子阱材料的价带结构，分析了用来展开的平面波的数目和周期对能量本征值的影响. 在实际计算中，平面波的周期必须选择足够大以保证包络函数在边界处消失，同时平面波的数目必须足够多以保证计算结果达到预定的精度.

关键词：半导体光放大器；应变量子阱；平面波展开方法；偏振

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