Hole subbands in semiconductor thin layers

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The hole subbands in an isolated thin layer are calculated by solving a 4×4 Luttinger-Kohn Hamiltonian numerically. We found that ignoring the warping of the valence band could lead to substantial error in the hole subbands and the related physical quantities, such as the effective masses. The normalized wave functions are presented.

A general formalism for space quantization of the energy spectrum for the valence band in semiconductor films has been proposed by Nedorezov.[1] To study this problem, he started from the Luttinger-Kohn Hamiltonian[2] in the spin $J=\frac{3}{2}$ basis by assuming infinite spin-orbit interaction, and imposed the zero boundary conditions that are valid for describing free carriers confined to an infinitely deep well. The subband structure of the valence band and the corresponding effective mass of the hole were derived analytically.[1] Recently, Fasolino and Altarelli[3] adopted Nedorezov's formalism to study the subband structure and Landau levels in heterostructures by neglecting the warping of the valence band. In the spirit of Ref. 3, and neglecting the warping of the valence band, Chang[4] studied the problem of the enhancement of optical nonlinearity in p-type semiconductor quantum wells due to confinement and stress.

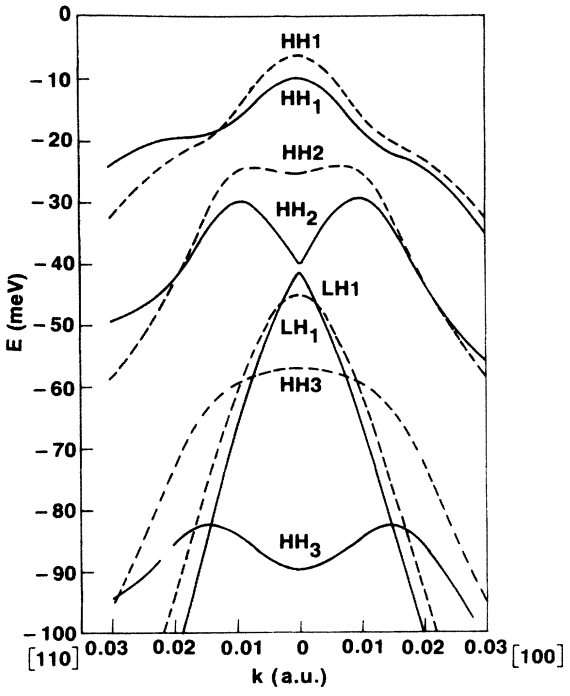

FIG. 1. Valence-band structure of the 100-Å GaAs single layer with $\gamma_1=6.85$, $\gamma_2=2.1$, and $\gamma_3=2.9$ (solid curves); and $\gamma_1=6.85$, $\gamma_2=2.58$, and $\gamma_3=2.58$ (dashed curves).

The main purpose of this paper is to investigate numerically the subband structure, the effective mass of the hole, and the wave functions of the Luttinger-Kohn Hamiltonian for the valence band, including the contribution of the warping by using Nedorezov's formalism.[1] We compare our results with those obtained without the warping of the valence band.[3,4]

The 4×4 Luttinger-Kohn Hamiltonian[2] can be reduced to two 2×2 matrices by using a unitary transformation, as proposed by Broido and Sham[5] and is written in atomic units (a.u.) as

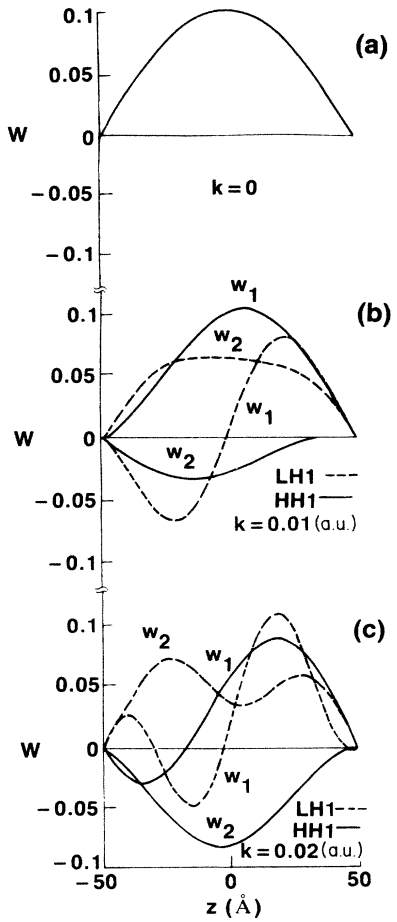

FIG. 2. Normalized wave functions $W_1(z)$ and $W_2(z)$ for typical k values.

$$\begin{bmatrix} P+Q-E & R-iS & 0 & 0 \\ R+iS & P-Q-E & 0 & 0 \\ 0 & 0 & P-Q-E & R-iS \\ 0 & 0 & R+iS & P+Q-E \end{bmatrix} \begin{bmatrix} W_1(z) \\ W_2(z) \\ W_3(z) \\ W_4(z) \end{bmatrix} = 0 , \tag{1}$$

where

$$\begin{aligned} P &= \gamma_1(k^2-\partial_z^2)/2 , \\ Q &= \gamma_2(k^2+2\partial_z^2)/2 , \\ R &= \{3k^4[\gamma_2^2\cos^2(2\theta)+\gamma_3^2\sin^2(2\theta)]/4\}^{1/2} , \\ S &= \sqrt{3}\gamma_3 k(-i\partial_z) . \end{aligned} \tag{2}$$

Here, γ_1, γ_2, and γ_3 are Luttinger parameters, $\mathbf{k}$ is the wave vector parallel to the layer in the (x,y) plane, i.e., normal to the direction z of the quantization of angular momenta, θ is the angle between $k_x\hat{\mathbf{x}}$ and $\mathbf{k}$, and ∂_z is the partial differential operator with respect to z. The zero boundary conditions require that

$$W_i(z=\pm L/2)=0, \quad i=1,2,3,4 , \tag{3}$$

where L is the thickness of the layer.

By examining Eqs. (1) and (2), we see that $W_4(z) \propto W_1^*(z)$ and $W_3(z) \propto W_2^*(z)$; therefore, we need only solve Eq. (1) for $W_1(z)$ and $W_2(z)$ with the boundary conditions Eq. (3). For GaAs, we choose[6] $\gamma_1=6.85$, $\gamma_2=2.1$, and $\gamma_3=2.9$. The numerical solutions for the eigenenergies E as a function of $\mathbf{k}$ in the [100] and [110] directions are shown as solid curves in Fig. 1 for $L=100$ Å. If we neglect the warping of the valence band as proposed by Ref. 3 by letting $\gamma_2=\gamma_3=\bar{\gamma}$ and $\bar{\gamma}=(3\gamma_3+2\gamma_2)/5=2.58$, we have been able to reproduce the energy spectrum obtained by Chang,[4] and show these results as the dashed curves in Fig. 1. The symbol HHn (LHn) refers to the heavy hole (light hole) in the nth state. Clearly, we see that by ignoring the warping of the valence band, the subband structure may have a large error which can possibly lead to misleading conclusions for the related physical quantities, such as effective masses. With warping (without warping) of the valence band, the effective masses are

$$\begin{aligned} m^*(\mathrm{HH1}) &= -0.14057 \ (-0.12306) , \\ m^*(\mathrm{HH2}) &= 0.00643 \ (0.2850) , \\ m^*(\mathrm{HH3}) &= 0.16542 \ (-0.71230) , \\ m^*(\mathrm{LH1}) &= -0.00603 \ (-0.06896) , \\ m^*(\mathrm{LH2}) &= -0.06207 \ (-0.06346) , \\ m^*(\mathrm{LH3}) &= -0.03018 \ (0.002936) . \end{aligned}$$

The numerical solutions of the normalized wave functions $W_1(z)$ and $W_2(z)$ for various $\mathbf{k}$ in the [100] direction with $n=1$ are shown in Fig. 2. In Fig. 2(a), we obtained exactly $W_{1,2}(z)=\sqrt{2/L}\cos(\pi z/L)$ and $W_{2,1}(z)=0$ for $k=0$. In this case, off-diagonal elements in Eq. (1) are zero, implying that $W_1(z)$ and $W_2(z)$ are decoupled. However, when $k\neq 0$, $W_1(z)$ and $W_2(z)$ are coupled because of the presence of the off-diagonal elements. Results are shown in Figs. 2(b) and 2(c) for $k=0.01$ and 0.02, respectively, a normalization condition

$$\int_{-L/2}^{L/2} dz[\,|W_1(z)|^2+|W_2(z)|^2]=1$$

having been employed. In these cases, we see that the spatial distributions of the heavy hole and the light hole in the layer are asymmetric.

In summary, we have investigated numerically Nedorezov's formalism for the space quantization of the energy spectrum for the valence band in a semiconductor thin layer. We have found that neglecting the warping of the valence band could lead to a large error in the subband structure and the related physical quantities.

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