Competition between the pseudomorphic strain mechanism with the piano-keyboard effect on the effective potential profile for coupled holes in layered heterostructures

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Formulation of the Problem

Several new features in the metamorphosis of the standardized fixed-height $V_{\text{eff}}$ profile for holes, in the presence of gradually increasing valence-band mixing and biaxial pseudomorphic strain, are presented. In some III – V unstrained semiconducting layered heterostructures a fixed-height potential, is not longer valid for lh. Indeed, we found –as predicted for electrons, permutations of the $V_{\text{eff}}$ character for lh, that resemble a “keyboard”, together with band offset changes, whenever the valence-band mixing varies from low to large intensity. Meanwhile for strained heterostructures, the former behavior, had been also detected for hh. Strain is able to diminish the keyboard effect on $V_{\text{eff}}$, and also makes it emerge or vanish occasionally. We found that multiband-mixing effects and stress induced events, are competitors mechanisms that can not be universally neglected by assuming a fixed-height rectangular spatial distribution for fixed-character potential energy, as a reliable test-run input for heterostructures.
The problem of quantum transport of charge carriers (electrons and holes) is narrowly linked to the study of spectral properties in heavy and light hole tunneling in semiconductor quantum heterostructures, as the appreciation of the fundamental transport properties of these materials can be directly applied to the analysis, design and functioning of practically all device structures that are currently technologically important. For many actual practical solutions and technological applications, due to the impressive development of low-dimensional electronic and optoelectronic devices, it is drastically important to include the valence-band mixing,[1] i.e. the degree of freedom transverse to the main transport direction, whenever the holes are involved. This phenomenology, early quoted by Wessel and Altarelli in resonant tunneling [2], has been lately pointed up for real-life technological devices.[1] If the electronic transport through these systems, engage both electrons and holes, the low-dimensional device response depends on the slower-heavier charge-carrier’s motion through specific potential regions.[3] It is unavoidable to recognize that in the specialized literature there is plenty of reports studying several physical phenomena derived from hole mixing effects, via standard existing methods.

However, just a few reports are available, concerning the evolution of the effective potential, as a central topic of investigation. Earliest striking elucidations due to Milanović and Tjapkin for electrons,[4] and recalled much later by Pérez-Álvarez and García-Moliner for a fully unspecific multiband theoretical case,[5] are fundamental cornerstones in this concern. The metamorphosis of the effective band offset potential $V_{\text{eff}}$, “felt” by charge carriers depending on the transverse momentum value, is so far, the better way to graphically mimic, the phenomenon of the in-plane dependence of the effective mass, also refereed as the valence-band mixing for holes. This is essentially the case of the carriers’ transverse motion connection with the $V_{\text{eff}}$ they interact with and is the main porpoise under investigation here. We assume the last widely understood as crucial, for charge and spin carriers’ quantum transport calculations through standard quantum barrier (QB) – quantum well(QW) layered systems.
On general grounds, $V_{\text{eff}}$ is given by the difference for 3D band edge levels as long as the transverse momentum ($\kappa_T$) values are negligible.[5] For finite $\kappa_T$, this assertion is no longer valid and the mixing effects reveal. The mechanism responsible for this behavior, is the increment of the $\kappa_T$-quadratic proportional term, yielding even to invert the roles of QW and QB. [4,5] Some authors had declared a shift upward in energy, of the bound states in the effective potential well as the transverse wave vector increases.[7] By letting grow $\kappa_T$, were found the valence-band mixing effects to arise and $V_{\text{eff}}$ to change.[8] They conclude a larger reduction for $V_{\text{eff}}$ as a function of $\kappa_T$, for light holes ($lh$) respect to that for heavy holes ($hh$).[8] Recently, a valence-band mixing first-principle theory within the envelope function approximation (EFA) was proposed, which had approximated the superlattice potential energy by considering only the linear and quadratic responses to the heterostructure perturbation.[6] These former works,[4,5,7,8,6] were motivating enough and put us on an effort to try a more comprehensive vision, of how $V_{\text{eff}}$ evolves spatially with $\kappa_T$ for $hh$ and $lh$. This section is devoted to demonstrate, the feasibility of a $V_{\text{eff}}$ profile evolution, as a reliable follow-up tool for finding the response of a layered semiconductor system —with spatial-dependent effective mass—, on travelling holes throughout it, by tuning the valence-band mixing and including strain effects.

The outline for this work is the following: We presents briefly the theoretical framework to quote valence-band $V_{\text{eff}}$ for both unstressed and stressed systems. Graphical simulations on $V_{\text{eff}}$ evolution, are exposed [9]. We exercise and discuss highly specialized $III - V$ semiconductor binary(ternary)-compound cases, that support the main contribution of the present study and suggest possible applications.
The movement equation of multiband systems, invariant in the presence of plane shifts \([x, y]\), has the following form [10]:

\[
\frac{d}{dz} \left[ B(z) \frac{dF(z)}{dz} + P(z)F(z) \right] + Y(z) \frac{dF(z)}{dz} + W(z)F(z) = O_N,
\]

where \(B(z)\) and \(W(z)\) are, in general, \((N \times N)\) Hermitian matrices and is fulfilled \(Y(z) = -P^\dagger(z)\).

Quadratic Eigenvalue Problem (QEP) [7, 11, 12]:

\[
Q(k_z)\Gamma = \{k_z^2\mathcal{M} + k_z\mathcal{C} + \mathcal{K}\}\Gamma = O_N,
\]

\[
\mathcal{M} = \begin{pmatrix}
-m^*_{hh} & 0 & 0 & 0 \\
0 & -m^*_{lh} & 0 & 0 \\
0 & 0 & -m^*_{h} & 0 \\
0 & 0 & 0 & -m^*_{hh}
\end{pmatrix}
\]

where

\[
\mathcal{M} = -B, \quad \mathcal{C} = 2iP \quad \text{and} \quad \mathcal{K} = W.
\]

\[
\det [Q(k_z)] = q_0k_z^8 + q_1k_z^6 + q_2k_z^4 + q_3k_z^2 + q_4,
\]
The operator $\hat{W}_{\text{eff}}$ for the effective band offset potential [8, 12]:

$$
\hat{W}_{\text{eff}} = \begin{pmatrix}
W_{11} & W_{12} & 0 & 0 \\
W_{12}^* & W_{22} & 0 & 0 \\
0 & 0 & W_{22} & W_{12} \\
0 & 0 & W_{12}^* & W_{11}
\end{pmatrix}
$$

(6)

$$
[\hat{W}_{\text{eff}} - V_{\text{eff}}I_4] \Psi(z) = O_4,
$$

(7)

At zero valence-band mixing, one has:

$$
V(z) = \begin{cases}
0 ; & z < z_l \\
V_b - V_a = V_{\text{eff}} ; & z_l < z < z_r \\
0 ; & z > z_r
\end{cases}
= \Theta V_{\text{eff}},
$$

(8)

The effective potential operator $\hat{W}_{\text{eff}}$ in the presence of biaxial strain [14]:

$$
\tilde{W}_{\text{eff}} = \hat{W}_{\text{eff}} + U_s I_4,
$$

(9)

Where the accumulated strain energy resulting:

$$
U_s = -\{a_v(2\varepsilon_1 + \varepsilon_3) + b(\varepsilon_1 - \varepsilon_3)\},
$$

(10)
To gain some insight into the rather complicated influence of the band mixing parameter $\kappa_T$, on the effective band offset, we display several graphics in the present section. The central point here, is a reliable numerical simulation for the spatial distribution of $V_{\text{eff}}$ while the valence-band mixing increases from $\kappa_T \approx 0$ (uncoupled holes) to $\kappa_T = 0.1\text{Å}^{-1}$ (strong hole band mixing).
Figure 1. (Color online) Panel (a)/(c) displays a cut of the $V_{eff}$ profile for $lh/hh$ (red/blue lines), at the interface plane between left and middle layers, as a function of $\kappa_T$. Panel (b)/(d) shows the progression of the band offset at the same interface for $lh/hh$ (red/blue lines), i.e. the difference between the upper-edge and lower-edge of the $V_{eff}$ profile. We have considered a GaP/AlN/GaP stress-free layered heterostructure.
Numerical Results and Discussion

In Figure 2, the $V_{\text{eff}}$ valence-band mixing dependence, exhibits a neatly permutation of the $V_{\text{eff}}$ character as the one predicted for electrons [12]. This permutation pattern is what we call as “keyboard" effect, and was detected for $lh$ only in stress-free systems. This strike interchange of roles for QB-like and QW-like layers, whenever the in-plane kinetic energy, varies from low to large intensity, represents the most striking contribution of the present study.

**Figure 2.** Panel (a) displays a cut of the $V_{\text{eff}}$ profile for $lh$ (red line), at the interface plane between left and middle layers, as a function of $\kappa_T$. Panel (b) shows the progression of the band offset, at the same interface for $lh$, i.e. the difference between the upper-edge and lower-edge of the $V_{\text{eff}}$ profile. We have considered a InAs/AlSb/InAs stress-free layered heterostructure.
Turning now to built-in elastic stressed layered heterostructures, we are interested to answer a simple question: whether or not the existence of a pseudomorphic strain becomes a weak or a strong competitor mechanism, able sometimes just to diminish the *keyboard* effect on $V_{\text{eff}}$, or even make it rises/vanishes occasionally. Figure 3 exhibits an unexpected *keyboard* effect risen for $lh$ in a $\text{InP:GaP/AlSb/GaP}$ layered heterostructure under a pseudomorphic strain, in comparison with a stress-free heterostructure. This evidence encourages to suggest $U_s$ (10), as a trigger mechanism in the presence of valence-band mixing to influence on $V_{\text{eff}}$.

**Figure 3.** (Color online) Panel (a) displays the 3D-perspective evolution of the stress-free $V_{\text{eff}}$ profile for $lh$ as $\kappa_T$ and layer dimension grow. Panel (b) shows the same for a $\text{InP:GaP/AlSb/GaP}$ strained layered heterostructure.
Conclusions

We present an alternative procedure to simulate graphically, the phenomenon of the transverse degree of freedom influence together with biaxial tensile strain impact on the effective scattering potential.

i) For low-intensity valence-band mixing regime, a fixed-height rectangular distribution of the potential-energy, is a good trial as a standard reference frame, for a theoretical treatment involving both flavors of holes under study. However this assertion is no longer valid, whenever the mixing effects reveal.

ii) At variance with the opposite for $hh$, the $lh$ exclusively, experience the striking \textit{keyboard} effect and permutations of $V_{\text{eff}}$ in stress-free systems. Nevertheless, in strained heterostructures, the former behavior, had been also found for $hh$.

iii) Evidences of this sort, mediated by $hh$-$lh$ coupling and strain, foretell their usefulness in experimental applications, valence-band profile tuning, valence-band offset manipulation and in theoretical analysis of hole tunneling.

iv) Pseudomorphic strain is able to diminish the \textit{keyboard} effect on $V_{\text{eff}}$, and also makes it emerge or even vanish eventually.

v) We conclude that the multiband-mixing effects modulated by stress induced events, are competitors mechanisms that can not be universally neglected by assuming a fixed-height rectangular spatial distribution for fixed-character potential energy, as a reliable test-run input for semiconducting heterostructures.
References