Inter-band coupling in Empirical Pseudopotential Method based bandstructure calculations of group IV and III-V nanostructures

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***Abstract*—This paper presents a systematic analysis of the use of the linear combination of bulk bands based on the empirical pseudopotential method to obtain the bandstructure of confined nanostructures. The relevance of interband coupling between conduction and valence bands in III-V materials is highlighted.**

***Index Terms*—Empirical pseudopotentials, linear combination of bulk bands, InAs, Ge, Si, bandstructure.**

I. INTRODUCTION

The introduction of new materials and very strongly confined nanostructures (FDSOI, FinFETs, nanowires) in CMOS technologies demands the development of full-zone bandstructure models with few empirical parameters and high physical accuracy [1], [2], [3]. The linear combination of bulk band (LCBB) approach based on the local empirical pseudopotentials model (EPM) is a flexible and efficient option due to its well recognized ability to simulate group IV and III-V materials, confined systems, arbitrary crystal orientations and strain configurations [4], [5], [6]. Full band models are particularly appropriate when dealing with high field transport in nanostructured devices, where multiple valleys contribute to the transport. In this paper, we use the LCBB model to study the importance of the interband coupling between conduction and valence bands in nanostructures consisting of Si, Ge and III-V materials.

II. MODEL

We will embrace a single material approximation where the confinement induced by a semiconductor-oxide heterostructure is described using appropriate discontinuities of conduction (CB) and valence band (VB). The LCBB method relies on the completeness of the Bloch states $|n, \mathbf{k}k_z\rangle = e^{i(\mathbf{k}\cdot\mathbf{r}+k_z z)}u_{n,\mathbf{k}k_z}$ of the underlying bulk crystal (with $u_{n,\mathbf{k}k_z}$ being the periodic part of $|n, \mathbf{k}k_z\rangle$), and writes the unknown wave-function of a confined system as a linear combination of $|n, \mathbf{k}k_z\rangle$ with coefficients $A_{n\mathbf{k}k_z}$ [4], [5], [6]. In the remainder of the paper we refer to a 2D electron gas and use z for the confinement direction. The secular equation for any in-plane wave-vector $\mathbf{k}$=(k_x,k_y) and band index n reads [6]

$$E_{n\mathbf{k}k_z} A_{n\mathbf{k}k_z} + \sum_{n',k'_z} M(n\mathbf{k}k_z, n'\mathbf{k}k'_z) A_{n'\mathbf{k}k'_z} = \varepsilon(\mathbf{k}) A_{n\mathbf{k}k_z} \tag{1}$$

where $E_{n\mathbf{k}k_z}$ is the energy corresponding to the bulk crystal state $|n\mathbf{k}k_z\rangle$, while $\varepsilon(\mathbf{k})$ describes the energy of the 2D electron gas. The matrix elements are defined as

$$M(n\mathbf{k}k_z, n'\mathbf{k}k'_z) = \langle n\mathbf{k}k_z|V_{n'}\Theta(z)|n'\mathbf{k}k'_z\rangle,$$

where $\Theta(z)$ is a unitary step function along the quantization direction z, such that $\Theta(z)$=0 for $|z|\leq T_{sct}/2$ and $\Theta(z)$=1 otherwise (with T_{sct} being the semiconductor film thickness). The potential energy $V_{n'}$ is either V_{cb} or V_{vb} respectively for n' being a conduction or a valance band. In a semiconductor-oxide system V_{cb} is positive whereas V_{vb} is negative, making impossible to describe the confining operator as a local potential in real space [7], [8].

The solution of Eq. (1) should be carried out by including the four VBs and the two or three lowest CBs of the underlying bulk crystal. We refer to this approach as the coupled solution of Eq. (1).

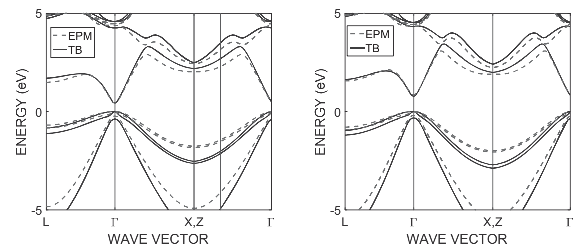

Fig. 1: Bandstructures obtained with the EP and the TB model for bulk (left) InAs and (right) $In_{0.53}Ga_{0.47}As$. Parameters are from Ref. [9] for the EPM and from Ref. [10] for the TB model.

A simplified and computationally lighter problem can be obtained if, for example, the conduction band of the 2D electron gas is studied by including in Eq. (1) only the CBs of

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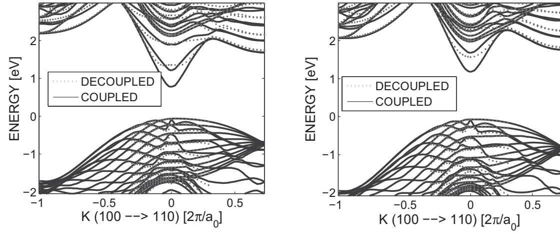

Fig. 2: Bandstructures obtained by using either the coupled or the decoupled LCBB model for (left) a InAs well with T_{sct}= 3.48 nm and (right) a $In_{0.53}Ga_{0.47}As$ well with T_{sct}= 3.37 nm. Confinement direction is (001).

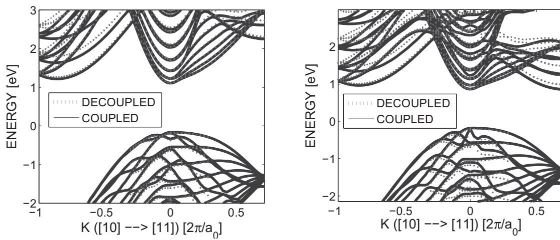

Fig. 3: Bandstructures obtained by using either the coupled LCBB or the decoupled LCBB model for (left) a Si film with T_{sct}= 3.12 nm and (right) a Ge film with T_{sct}= 3.25 nm. Confinement direction is (001).

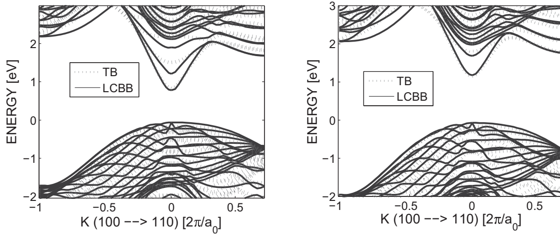

Fig. 4: Bandstructures obtained by using either the coupled LCBB or the TB model for (left) a InAs film with T_{sct}= 3.48 nm and (right) a InGaAs film with T_{sct}= 3.37 nm. Confinement direction is (001).

the bulk crystal. This approach neglects the possible coupling between the bulk crystal VBs and CBs, and we will refer to it as decoupled solution of Eq. (1). While the decoupled solution is a good approximation for indirect bandgap materials like Si having a relatively large, indirect energy gap, it is instead not justified in small-gap, direct bandgap semiconductors like InAs or InGaAs. This paper illustrates in detail the importance of such VB-CB coupling in III-V as opposed to group IV materials.

III. RESULTS

We start showing in Fig. 1 the good matching between the bulk bandstructures of InAs and $In_{0.53}Ga_{0.47}As$ obtained by using the EPM and the sp3d5s* tight-binding (TB) method [10], the latter method being used as reference throughout the paper. Very close band gaps at the Γ point are obtained with the two models.

Figure 2 illustrates the influence of the VB-CB coupling on the bandstructures of 2D quantum wells based on small-gap semiconductors such as InAs and InGaAs. A significant overestimation of the band-gap at the Γ point is found for the decoupled calculation. This discrepancy between the two models is not observed in group-IV semiconductors such as Si and Ge. In Fig. 3, for example, a very similar energy gap at the Γ point is observed in a Si quantum well for either coupled or decoupled calculations. This is a consequence of the large, indirect band-gap of Si and Ge bulk materials.

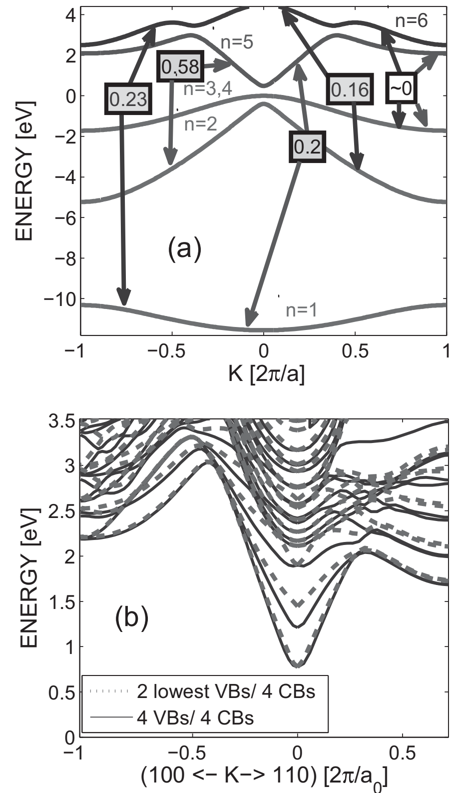

Fig. 5: (a) Bulk InAs bandstructure and values of some interband coupling $C^{n,n'}$ defined as in Eq. (2) between conduction and valence bands and calculated at **k**=0. (b) Conduction subbands of an InAs well with T_{sct}= 3.48 nm obtained with the LCBB method coupling the four lowest CBs either with the two lowest VBs or with all four VBs. Confinement direction is (001).

For Ge, however, the decoupled calculation predicts a similar value for the gap in Γ and L (i.e. 0.863 eV), while the coupled calculation suggests that the energy gap in L is significantly larger (0.99 eV) than the gap in Γ (0.863 eV). This emphasizes the importance of an inclusion of both CBs and VBs also for LCBB calculations in Ge based nanostructures.

Figure 4 further underlines that in III-V quantum wells it is mandatory to include the VB-CB coupling in the LCBB calculations in order to reproduce the TB results. Figure 5(a) provides a pictorial illustration and also a quantitative

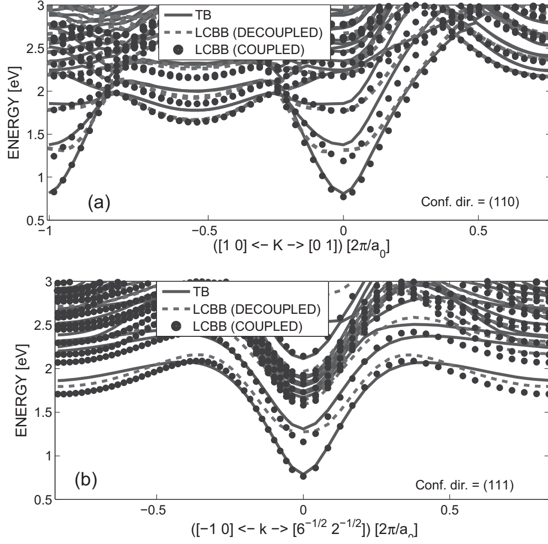

Fig. 6: Conduction subbands obtained by using the decoupled LCBB, the coupled LCBB and the TB model for an InAs film with confinement along (a) the (110) and (b) the (111) direction. T_{sct}= 3.48 nm.

evaluation of the interband coupling between the VBs and CBs of InAs. The coupling has been here defined as

$$C^{n,n'} = \sum_{k_z,k_z'} |S^{n,n'}_{k_z,k_z'}| / \sum_{k_z,k_z'} |S^{n',n'}_{k_z,k_z'}|, \tag{2}$$

where $S^{n,n'}_{k_z,k_z'}$=$\langle u_{n\mathbf{k}k_z} | u_{n'\mathbf{k}k_z'} \rangle$ is the overlap integral between the periodic parts of the Bloch states. Bulk bands are numbered as shown in Fig. 5(a), with n=1 being the lowest valence, and n=5 being the lowest conduction band. Interestingly, it is found that the most important coupling involves the CBs and the two lowest VBs (i.e. n=1, 2) instead of the two highest VBs, which is the picture that one may have expected. This is confirmed and further illustrated in Fig. 5(b) reporting the bandstructure of an InAs well with T_{sct}= 3.48 nm obtained with the LCBB method and considering the coupling of the CBs either with all four valence bands (i.e. n=1, 2, 3, 4) or with only the two lowest VBs (i.e. n=1, 2). The conduction subbands of the 2D gas are very similar in the two cases, thus confirming that the coupling between the CBs and the two lowest VBs (i.e. n =1, 2) is in fact dominant.

Remarkably, similar results about the importance of VB-CB coupling and the good agreement between the coupled LCBB and TB results are observed also for different confinement directions. This can be seen in Fig. 6 illustrating the lowest conduction subbands for an InAs well confined along the (110) and the (111) directions.

Finally, Fig. 7 reports the energy bandgap dependence on the well thickness of the various III-V-based quantum wells for both the coupled LCBB and the TB model. A fair agreement between the two models is observed for all materials and geometrical dimensions.

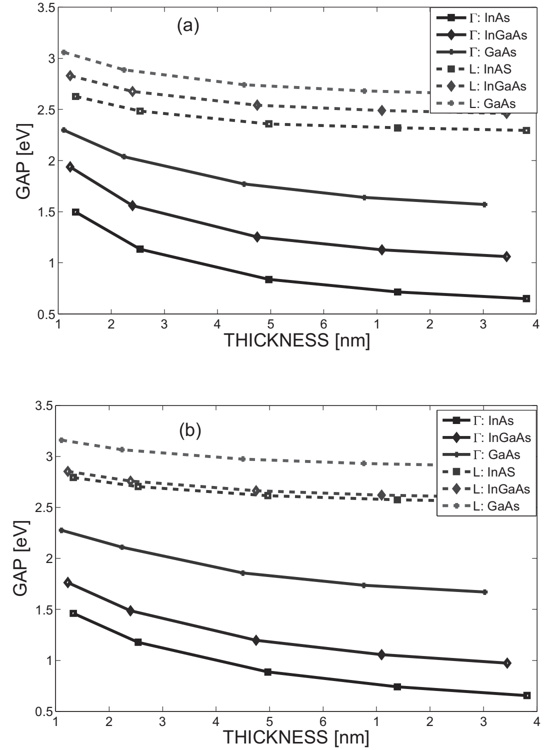

Fig. 7: Energy-gap evolution as a function of the layer thickness of various III-V films obtained by using (a) the coupled LCBB and (b) the TB model. Confinement direction is (001).

IV. Conclusion

The importance of including the coupling between the valence and the conduction bulk bands within the LCBB method has been comprehensively discussed by showing relevant examples of group IV and III-V nanostructures.

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