Modeling Study of Ultra-Thin Ge Layers Using Tight-Binding, LCBB and kp Methods

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Abstract

The confined states in ultra-thin Ge layers on oxide are investigated using three different state-of-the-art full-band methods. Contrary to the prediction of the simple effective mass approximation (EMA) and multiband-models that decoupled the Conduction Bands (CB) and the Valence Bands (VB), full-band calculations predicts much lower subband energy shifts due to quantum confinement.

1 Introduction

The semi-empirical computational methods for the calculation of the electronic energy band structure of a 2-D gas fall into two general categories. The tight-binding (TB) approach that has been extensively used to investigate the confined states in bulk semiconductors [1] uses an atomistic description of the layer. Alternatively, the linear combination of bulk bands (LCBB) method described in [2], the envelop function approximation [3] based on the full-zone kp analysis [4], and the effective-mass approximation uses a continuous description of the matter. In these later methods an effective confining potential is needed to account for the boundaries of the layer. In this work, a comparison between the TB approach, the LCBB, the kp and the EMA is presented. The importance of using a full-band description of the semiconductor is addressed quantitatively in the case of a thin Ge layer on oxide.

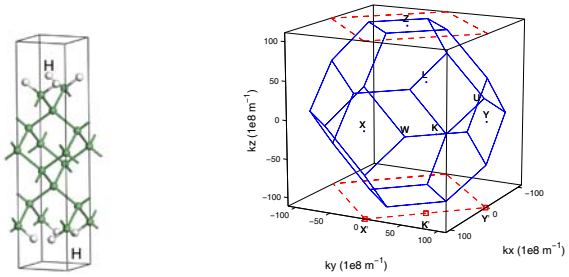

Figure 1: Left: super cell used in TB model for a [001]-oriented Ge layer in which the dangling bounds are passived with H. Right: three dimensional (blue lines) and two-dimensional (dashed red lines) Brillouin zone and high symmetry points in reciprocal space.

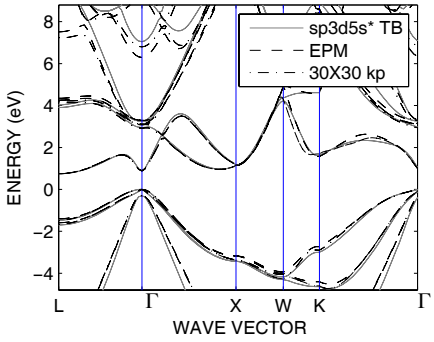

Figure 2: Bandstructure of bulk Ge along various directions in reciprocal space (see Fig 1) calculated using TB, EPM and full-zone kp methods.

2 Computational methods in 2-D semiconductors

(i) **Tight-Binding**: Using TB models it is a straightforward matter to work out the quantum properties of thin films using the supercell approach (see Fig 1) in which the surface dangling bounds are passived with Hydrogen (H) [1].

(ii) **LCBB**: Our calculations are based on the recently developed empirical pseudopotential-based LCBB method [2]. This method relies on the expansion of the confined states in terms of Bloch functions, solution to the 3-D crystal Hamiltonian. As proposed in [2], we used only the two lowest CBs to describe the electron confined states. Similarly, we used the three highest VBs to described the hole confined states.

(iii) **kp**: The present kp calculations are based on the envelop function approximation [3] that expand the confined states in terms of trigonometric functions. We compared the results obtained with this method using the 6-level Dresselhauss-Kip-Kittel kp model but also with the recently developed "full-zone" 30-level kp model [4].

Because the LCBB and the kp methods are not atomistic descriptions, there is no thorough way to provide a boundary potential consistent with TB boundary condition. Thus, in (ii) and (iii), as well as with EMA, the finite thickness of the layer is modeled using an infinite additional positive (negative) potential for the CBs (and the VBs), in such a way that the confined states do not extend outside the well.
The bulk Ge *fitting* parameters used in the present sp3d5s* TB, 30-level kp and nonlocal relativistic EPM were fitted on reference abinitio Density-Functional Theory simulations following the optimization procedure shown in [4] and [5]. A very close agreement between these three methods was obtained (as it is testified in Fig. 2). This ensure a meaningful comparison of the present calculations of the confined states in ultra-thin Ge layers of various thickness.

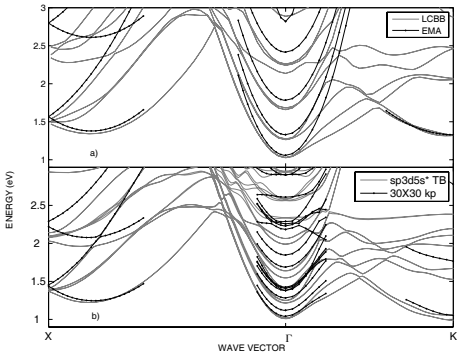

Figure 3: Electron confined bandstructure of a 2.26 nm [001]-Ge layer calculated using a) LCBB and EMA, and b) 30-level kp and sp3d5s* TB models.

3 Ge Electronic sub-structure and confinement energies

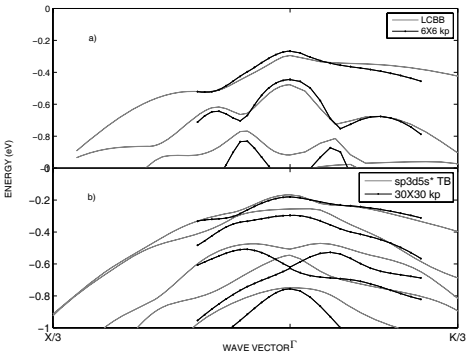

Figure 4: Same as Fig 3, but for the Holes.

In Figs. 3 and 4 the CBs and VBs sub-structure obtained using TB is superimposed to the 'full-zone' kp results for a 2.26nm thick layer. Also shown, are the LCBB results and the EMA results for electrons and 6-level kp ones for holes (Fig. 4). As can be seen (in Figs. 3 b and 4 b), the energy sub-structure calculated using the TB and the full-band kp methods are similar (indirect $\Gamma - L$ gap), but significantly different (Figs. 3 a and 4 a) to the LCBB, 6-level kp and EMA results (direct gap). One notes nevertheless, that the electronic sub-structures obtained using these methods superimpose remarkably well.
The extracted CBs and VBs energy shifts are shown in Fig. 5 as a function of layer thicknesses. Due to a much smaller quantization mass for the Γ and L-valleys, a simple EMA calculation predicts that these valleys would be uplifted above the competing Δ-valleys. As seen, this is also the case with the present LCBB solutions, in which

only a limited number of bands are considered. As previously, one notes a very close agreement between the band shifts obtained using these two later methods, which is consistent with the results reported in [2]. Similarly, when the LCBB method is applied to holes (taking into account in the calculation only the three upmost VBs), one obtains results that are similar to the 6-level kp ones (that also consider only the three upmost VBs), but different to the Tb and the kp results.

4 Conclusion

The electronic sub-band structure of thin semiconductor layers has been investigated using several computational methods. We conclude from the previous analysis that in Ge a considerable amount of coupling between the CB and the VBs, render the EMA, the 6-level kp and the uncoupled LCBB approach unreliable in ultra-thin layers. Similar studies in Si layers (not shown here), have shown a much better agreement between the predictions of these methods, even in very thin layer (2 nm). Due to larger gaps in Si than in Ge, the coupling between the CBs and VBS is less pronounced, and it is possible in the calculation to consider only a limited number of bands.

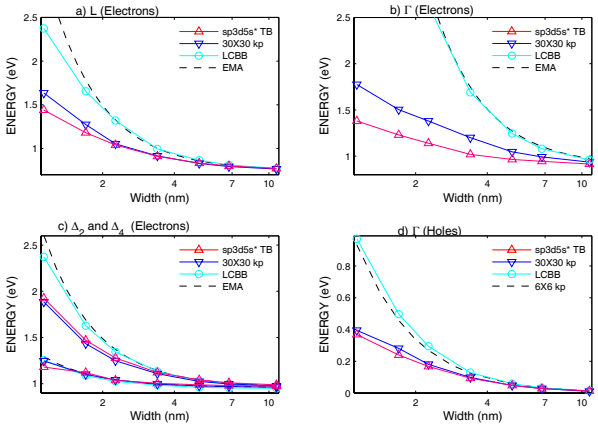

Figure 5: Calculated energy shifts of the first Ge electron subband for a) L-valleys, b) Γ -valley, c) Δ_2 and Δ_4-valleys, and d) for the Holes. Calculation have been performed for various thicknesses using sp3d5s* TB, 30-level kp, 6-level kp, LCBB and EMA methods.

References

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