

Validity of the Effective Mass Approximation in Silicon and Germanium Inversion Layers

J.L. van der Steen, D.Esseni*, P.Palestri*, L.Selmi*

MESA+ Institute for Nanotechnology, University of Twente, Enschede, The Netherlands

* DIEGM, University of Udine, Via delle Scienze 208, 33100 Udine

INTRODUCTION

The electron device community is actively investigating transistors realized in Ultra-Thin (UT) semiconductor films. The Effective Mass Approximation (EMA) is very frequently used to describe the nano-MOSFETs [1], however a comparison with more rigorous bandstructure calculations is highly demanded [2]. In this paper we use the method of the Linear Combination of Bulk Bands (LCBB) to calculate the band structure in UT silicon and germanium nano-transistors and compare the eigenvalues, energy dispersion and density of states (DOS) with the simplified EMA results

LCBB AND EMA QUANTIZATION MODELS

In the LCBB quantization model the *unknown* wavefunction is expanded in terms of the Bloch functions $\Phi_{n\mathbf{k}k_z}$ of the underlying crystal [3], [4], where n is the band of the Bloch function, \mathbf{k} denotes the in-plane wavevector, and z is the quantization direction. By selecting an appropriate set of k_z values it is possible to obtain a separated eigenvalue problem for each in-plane \mathbf{k} [4], the resulting energy dispersion for Si(111) is illustrated Fig.1.

In the EMA approach, a *single* Schrödinger-like equation in the real space is solved for each valley [5]. The set of EMA parameters used in this work are reported in Tab.I and are derived from [6].

RESULTS AND DISCUSSION

The confining potential used for both EMA and LCBB calculations is a squared well with a width of T_{SCT} and a barrier of $\Phi_B=3eV$, hence the penetration of the wavefunction in the oxide is accounted for. Fig.2 reports the lowest eigenvalue versus T_{SCT} for the $D_{0.916}$ and the $D_{0.19}$ valleys of Si(100). The EMA tracks the LCBB results very well. With an infinite barrier, instead, the EMA

eigenvalues increase well above the LCBB values at the smallest T_{SCT} . Fig.3 reports the same comparison as in Fig.2 for the $L_{0.219}$, the $D_{0.33}$ and the Γ valleys in Ge(110). Even in this case the EMA reproduces the absolute and relative position of the valleys indicated by the LCBB model.

Fig.4 reports the energy dispersion for Si(111) along the dashed line indicated in Fig.1. According to the position of the minima in the 3D Brillouin Zone (BZ), the EMA predicts a minimum at $k_x=1.7/\sqrt{6}(2\pi/a_0)\simeq 0.6940(2\pi/a_0)$. The LCBB results do exhibit such a minimum for relatively large T_{SCT} values (not shown). However, Fig.4 shows that for $T_{SCT}=2nm$ the minimum of the LCBB bandstructure tends to move at the edge of the 2D BZ (i.e. at $k_x=2.0/\sqrt{6}(2\pi/a_0)\simeq 0.8165(2\pi/a_0)$) thus creating a discrepancy between the EMA and LCBB results. The LCBB energy dispersion has a flat energy branch, whose effective mass is much larger than the $m_{le}=0.674$ value reported in Tab.I. This feature of the LCBB calculations result in a large DOS at the very bottom of the conduction subbands (see Fig.5), that decreases with the increase of the energy.

As illustrated in Fig.4, we found that the LCBB and EMA 2D energy dispersion can be quite different at the smallest T_{SCT} . Thus, the LCBB method has been used to calculate T_{SCT} dependent transport masses, that will be discussed at the conference. **Acknowledgment:** This work was partially supported by the Italian MIUR (PRIN 2004) and by the EU (SINANO NoE, IST-506844).

REFERENCES

- [1] S.E. Laux. in *IEDM Technical Digest*, p.135, 2004.
- [2] A.Rahman *et al.* in *IEDM Technical Digest*, p.139, 2004.
- [3] F.Chirico *et al.* in *Phys.Rev.B*, **64**, p.045314, 2001.
- [4] D.Esseni *et al.* in *Phys.Rev.B*, **72**, p.165342, 2005.
- [5] C.Jungemann *et al.* in *Solid State Electr.*, **36**, p.1529, 1993.
- [6] F.Stern *et al.*, *Physical Review* **163**, 816-835 (1967).

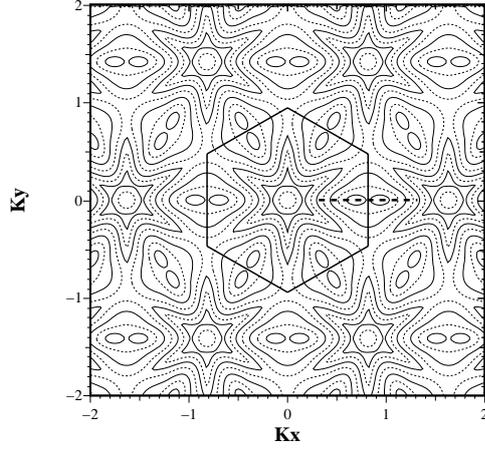


Fig. 1. Si(111), $T_{SCT}=5nm$. Lowest eigenvalue vs. \mathbf{k} obtained with the LCBB method. The six degenerate minima are in $\mathbf{k}=(\pm 1.7/\sqrt{6}, 0)$ and in $\mathbf{k}=(\pm 0.85/\sqrt{6}, \pm 0.85/\sqrt{2})$. The hexagon indicates the 2D Brillouin zone [4].

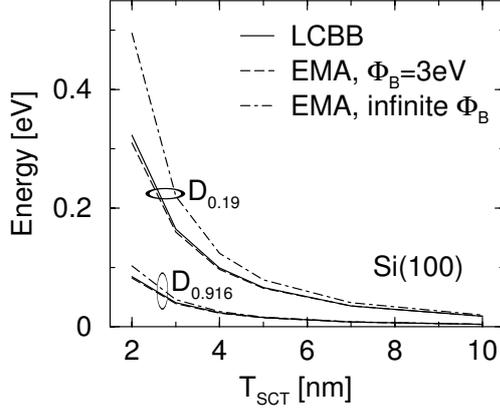


Fig. 2. Si(100). Lowest eigenvalue versus T_{SCT} for the $D_{0.916}$ and $D_{0.19}$ valleys calculated with either the LCBB or the EMA model. The infinite Φ_B EMA results are obtained by setting the wavefunction to zero at the oxide interface.

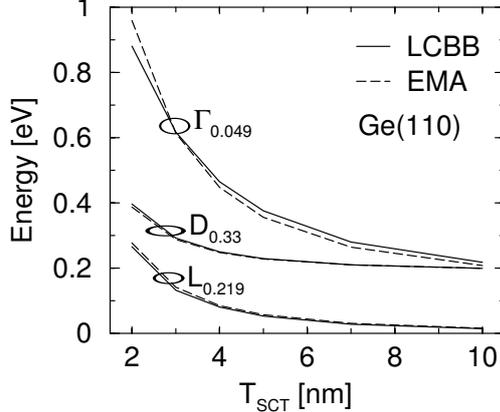


Fig. 3. Ge(110). Lowest eigenvalue versus T_{SCT} for the $L_{0.219}$, $D_{0.33}$ and $\Gamma_{0.049}$ valleys calculated with either the LCBB or the EMA model. The energy offset of the D and Γ valleys with respect to the L valleys of bulk germanium is assumed to be $189meV$ and $145meV$, respectively.

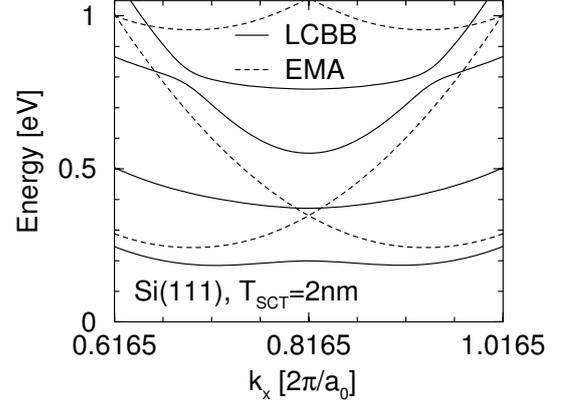


Fig. 4. Si(111), $T_{SCT}=2nm$. Energy dispersion along the dashed line indicated in Fig.1 obtained with either the LCBB or the EMA model. The minimum is at $k_x=1.7/\sqrt{6}(2\pi/a_0)$ according to the EMA model. The minimum in the LCBB model has both a different position and a different value.

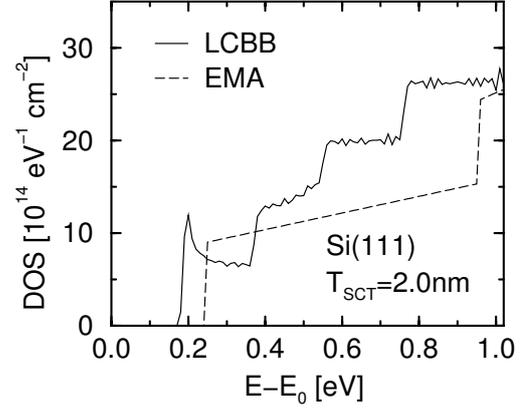


Fig. 5. Si(111), $T_{SCT}=2nm$. Density of states calculated with either the LCBB or the EMA model. A spike of DOS is observed in the LCBB results, which is produced by the flat energy branch in Fig.4. In the EMA model a non-parabolicity factor $\alpha=0.5eV^{-1}$ is used.

Material	m_{te}	m_{le}	m_z	n_ν	Label
Si(100)	0.190	0.190	0.916	2	$D_{0.916}$
	0.19	0.916	0.190	4	$D_{0.19}$
Si(111)	0.190	0.674	0.258	6	$D_{0.258}$
Ge(110)	0.080	0.600	0.219	2	$L_{0.219}$
	0.2	0.575	0.33	4	$D_{0.33}$
	0.049	0.049	0.049	1	$\Gamma_{0.049}$

TABLE I
DEGENERACY n_ν , QUANTIZATION MASS m_z AND EFFECTIVE MASSES m_{le} AND m_{te} ALONG THE PRINCIPAL AXES OF THE ELLIPSES THAT DESCRIBE THE IN-PLANE ENERGY DISPERSION IN THE EMA MODEL. THE PARAMETERS CORRESPOND TO THE DOMINANT VALLEYS FOR Si(100), Si(111) AND Ge(110) AND ARE CALCULATED AS EXPLAINED IN [6].