Comparative Analysis of Pseudo-Potential and Tight-Binding Band Structure Calculations with an Analytical Two-Band k·p Model: Conduction Band of Silicon

V. Sverdlov[1,2] , H. Kosina[1] , and S.Selberherr[1]

1. *Institute for Microelectronics, TU Wien, Wien, 1040 Austria, E-mail sverdlov@iue.tuwien.ac.at.*
2. *V.A. Fock Institute of Physics, State University of St.Petersburg, 198904 St.Petersburg, Russia.*

The **k·p** theory allows to describe the band structure analytically. After the pioneering work by Luttinger and Kohn [1] the six-band **k·p** method has become widely used to model the valence band in silicon. The conduction band in silicon is usually approximated by three pairs of equivalent minima located near the *X*-points of the Brillouin zone. It is commonly assumed that close to the minima the electron dispersion is well described by the effective mass approximation. A non-parabolicity parameter is introduced to describe deviations in the density of states from the purely parabolic expression, which become pronounced at higher electron energies. In ultra-thin body FETs, however, the non-parabolicity affects the subband energies substantially, and it was recently indicated that anisotropic, direction-dependent non-parabolicity could explain a peculiar mobility behavior at high carrier concentrations in a FET with (110) film orientation [2]. Therefore, and because of its inability to address properly the band structure modification under stress, a more refined description of the conduction band minima beyond the usual single-band non-parabolic approximation is needed.

A recently proposed two-band **k·p** model for the conduction band of silicon [3] is compared with other band structure models, notably the nonlocal empirical pseudo-potential method [4] and the $sp^3d^5s^*$ nearest-neighbor tight-binding model [5]. The two-band **k·p** model is demonstrated to predict results consistent with the empirical pseudo-potential method, and to accurately describe the band structure around the valley minima, including the effective masses and the band non-parabolicity. The tight-binding model, on the other hand, overestimates the gap between the two lowest conduction bands at the valley minima, which results in an underestimation of the non-parabolicity effects.

In biaxially stressed Si films the electron mobility can be nearly doubled [6]. The reason for the mobility enhancement lies in the stress-induced band structure modification. The degeneracy between the six equivalent valleys is lifted due to stress-induced valley shifts. This reduces inter-valley scattering. In case of tensile biaxial stress applied in the (100) plane the four in-plane valleys move up in energy and become de-populated. The two populated out-of-plane valleys have favorable conductivity masses, which together with reduced inter-valley scattering results in the observed mobility increase [7].

The technologically relevant uniaxial stress along [110] has received little attention in the research community and was systematically investigated experimentally just recently [8]. Inherent to [110] uniaxial stress, the shear distortion of the crystal lattice induces pronounced modifications in the conduction band. Contrary to biaxial stress, the electron mobility data for [110] stress suggest that the conductivity mass depends on stress. Any dependence of the effective masses on stress is neglected within the single-band description of the conduction band and can only be introduced phenomenologically. In order to describe the dependence of the effective mass on stress a single-band description is not sufficient, and coupling to other bands has to be taken into account.

The two-band **k·p** model gives analytical expressions for the shear strain-dependence of the band structure parameters. Shear strain modifies substantially both the longitudinal and transversal effective masses [3,8,9]. The transversal mass determines the mobility in FETs with ultra-thin body. In these FETs the electron mobility enhancement induced by [110] tensile stress is therefore solely caused by a decrease of the conductivity mass in the stress direction. Predictions of the two-band **k·p** model are in good agreement with those of the pseudo-potential method [10].

This work was supported in part by the Austrian Science Fund FWF, project P9997-N14.

1. J.M. Luttinger, W. Kohn, *Phys.Rev*. **97**, 869 (1955).
2. K. Uchida *et al.*, *IEDM* 2006, pp.1019-1021.
3. V. Sverdlov *et al.*, *EUROSOI* 2007, pp.39-40.
4. M.M. Rieger, P. Vogl, *Phys.Rev.B* **48**, 4276 (1993).
5. T.B. Boykin *et al.*, *Phys.Rev.B* **69**, 115201 (2004).
6. K. Rim *et al., VLSI Symp.* 2002, pp. 98-99.
7. S.I. Takagi *et al.* , *J.Appl.Phys*. **80**, 1567 (1996).
8. K. Uchida *et al.*, *IEDM* 2005, pp. 129-132.
9. J.C. Hensel *et al.*, *Phys.Rev*. **138**, A225 (1965).
10. V. Sverdlov *et al.*, *ESSDERC* Sept 2007.