Numerical Study of the Electron Subband Structure in Strained Silicon UTB Devices

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1. Abstract

A self-consistent Schrödinger-Poission model for the calculation of the electron subband structure is presented, taking into account the band nonparabolicity and shear strain based on a two-band $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian. Emphasis is put on the efficiency and accuracy of the numerical, two-dimensional $\mathbf{k}$-space integration by means of the Clenshaw-Curtis method. Simulation results of a Silicon ultra thin body double gate device demonstrate the suitability of the proposed numerical method for the calculation of the electron density.

2. Numerical Model

The numerical modeling of the electron subband structure in ultra thin body SOI MOS structures relies on an accurate description of the bulk Hamiltonian. In this work, we applied a two-band $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian [1, 2] describing the Silicon conduction band around the X points given by

$$\mathbf{H} = \begin{bmatrix} \mathrm{H}_- & \mathrm{H}_{\mathrm{bc}} \\ \mathrm{H}_{\mathrm{bc}} & \mathrm{H}_+ \end{bmatrix} \qquad \text{with}$$

$$\mathrm{H}_{\mp} = \mathcal{E}_{\mathrm{c}}(z) + \frac{\hbar^2 k_{\mathrm{z}}^2}{2m_{\mathrm{l}}} + \frac{\hbar^2\left(k_{\mathrm{x}}^2 + k_{\mathrm{y}}^2\right)}{2m_{\mathrm{t}}} \mp \frac{\hbar^2 k_0 k_{\mathrm{z}}}{m_{\mathrm{e}}},$$

$$\mathrm{H}_{\mathrm{bc}} = D\epsilon_{\mathrm{xy}} - \frac{\hbar^2 k_{\mathrm{x}} k_{\mathrm{y}}}{M}.$$

$\mathcal{E}_{\mathrm{c}}$ denotes the conduction band edge energy, m_{l} and m_{t} are the longitudinal and transversal electron masses, and $\frac{1}{M} \approx \frac{1}{m_{\mathrm{t}}} - \frac{1}{m_{\mathrm{e}}}$. The shear strain deformation potential $\mathrm{D} = 14\mathrm{eV}$ and the shear strain component ϵ_{xy} describe the effects of strain on the bandstructure. $k_0 = 0.15\frac{2\pi}{a}$ corresponds to the distance of the valley to the X point. The quantization is carried out by the replacement $k_{\mathrm{z}} \rightarrow -\mathrm{i}\,\partial_{\mathrm{z}}$. The Discretization is realized with symmetric operator ordering and application of a finite difference scheme with hard wall boundary conditions. The resulting eigenvalue problem gives rise to discrete energies describing the subband structure.
The contribution of subband i and valley j to the equilibrium electron concentration is given by

$$n_{i,j}(z) = |\psi_{i,j}(z)|^2 \int_{\mathrm{BZ}} \mathrm{d}^2\mathbf{k} \frac{1}{(2\pi)^2} f_0\left(\mathcal{E}_{i,j}\left(k_{\mathrm{x}}, k_{\mathrm{y}}\right), \mathcal{E}_{\mathrm{F}}\right),$$

where $\psi_{i,j}$ is the wave function and f_0 is the Fermi distribution which depends on the Fermi level $\mathcal{E}_{\mathrm{F}}$ and the dispersion relation $\mathcal{E}_{i,j}\left(k_{\mathrm{x}}, k_{\mathrm{y}}\right)$ of the subband. Therefore, to calculate the electron occupation of a subband a numerical, two-dimensional $\mathbf{k}$-space integration is required. Since this necessitates to solve the Schrödinger equation for every discrete point $(k_{\mathrm{x}}, k_{\mathrm{y}})$ one seeks after a numerical quadrature scheme that gives good accuracy on as few grid points as possible. Our first choice was the Clenshaw-Curtis method presented in [3]. For the integration interval $[-1, 1]$ it uses the zeros of the Chebyshev polynomial given by $x_k := \cos(k\frac{\pi}{n})$ with $k = 0, 1, \ldots, n$ as nodes. The weights are written explicitely as [4]

$$w_k = \frac{c_k}{n}\left(1 - \sum_{j=1}^{\lfloor n/2 \rfloor} \frac{b_j}{4j^2 - 1}\cos\left(2jk\frac{\pi}{n}\right)\right)$$

with $b_j = 1$ if $j = n/2$, or $b_j = 2$, if $j < n/2$, and $c_k = 1$ if $k \mod n = 0$, or $c_k = 2$ otherwise. An advantage of this method is the ability to use subsets of half the number of the nodes for a lower degree rule. This allows for adaptive numerical quadrature schemes which have proven suitable for energy domain integration as shown for the NEGF method in [5]. For the $\mathbf{k}$-space integration of the subbands provided by the two-band Hamiltonian excellent accuracy has been achieved with only 19 nodes per k direction. The integration intervals have been chosen as ten percent of the width of the Brillouin zone in each positive and negative direction. The sum given by the Clenshaw-Curtis rule has been normalized accordingly.

3. Results and Conclusion

To test the implemented $\mathbf{k}\cdot\mathbf{p}$ model a rectangular Silicon potential well with 5 nm width and the electron masses $m_{\mathrm{l}} = 0.91m_{\mathrm{e}}$ and $m_{\mathrm{t}} = 0.19m_{\mathrm{e}}$ has been simulated. Fig. 1 shows the numerically calculated dispersion relation of the first and second subband. Fig. 2 illustrates the influence of strain on the dispersion relation. The results are in good agreement with analytical considerations [6].

To properly incorporate the electrostatics in realistic devices a self-consistent Schrödinger/Poisson scheme

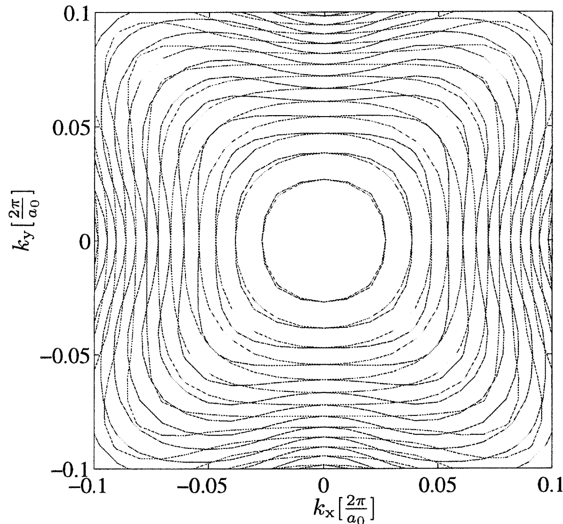

Fig. 1: *Dispersion relation of the lowest (red) and second (blue) subband of a 5 nm Silicon quantum well as contour plot in 20 meV steps.*

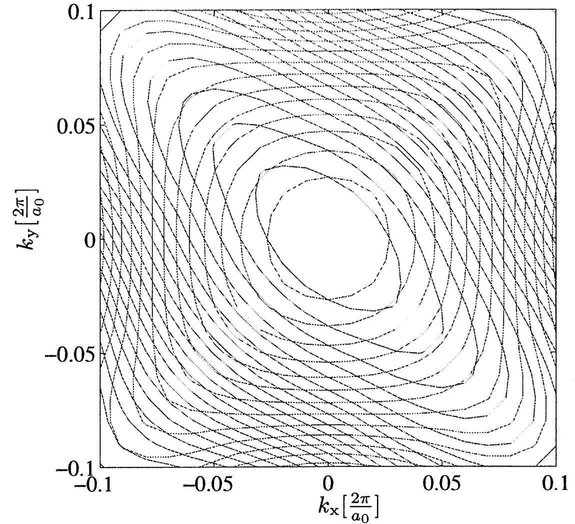

Fig. 2: *Dispersion relation of the lowest subband of a 5 nm Silicon quantum well with a strain of* $\epsilon_{xy} = 1\%$ *(blue) and without strain (red) as contour plot in 20 meV steps.*

has been employed. A Silicon ultra thin body DG-MOSFET with 3 nm film thickness and 1 nm oxide thickness has been simulated. The donor doping of the polysilicon gates was $N_D = 1.0 \times 10^{20}\,\text{cm}^{-3}$ and the Si film was lightly p-doped with $N_A = 2.0 \times 10^{16}\,\text{cm}^{-3}$. Fig. 3 shows the conduction band edge and the electron concentration provided by the simulation. Within the well the squared wave functions for the four lowest, twofold degenerate subbands are displayed at their corresponding energy levels. For each subband the electron occupation is calculated by **k**-space integration. The electron distribution of the lowest subband is depicted in Fig. 4. The grid lines are distributed according to the Clenshaw-Curtis method, which gives an accumulation of grid points at the boundary of the integration domain. Contrary to numerical solutions based on the one-band effective mass Schrödinger equation this work considers the nonparabolic dispersion relation. Furthermore, shear strain effects leading to a warping of the bandstructure are accounted for. These properties are crucial for transport models relying on subband calculations.

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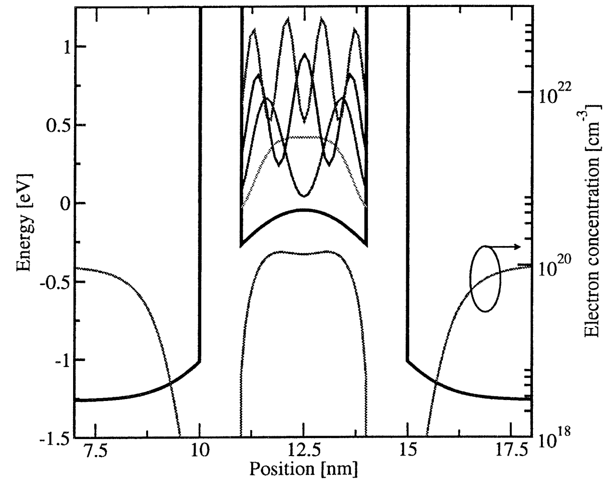

Fig. 3: *Self-consistent calculation of the conduction band edge and the electron concentration of a Si-DG-MOSFET with 3 nm well width and 1 nm oxide thickness. The normalized wave functions* $[nm^{-1}]$ *are overlayed at their respective energy niveaus.*

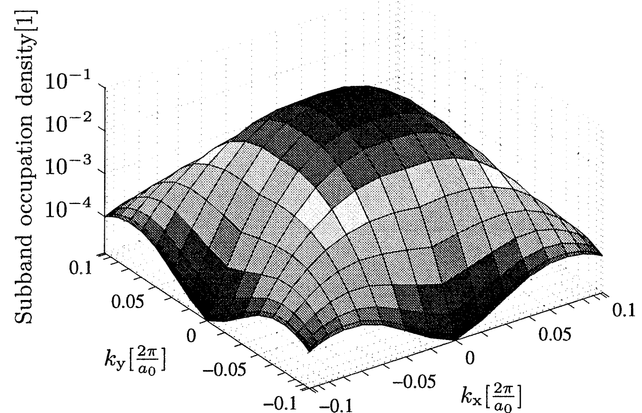

Fig. 4: *Occupation of the lowest subband of a 3 nm Silicon quantum well. The grid corresponds to the nodes of the numerical quadrature.*