TCAD ready density gradient calculation of channel charge for Strained Si/Strained $Si_{1-x}Ge_x$ dual channel pMOSFETs on (001) Relaxed $Si_{1-y}Ge_y$

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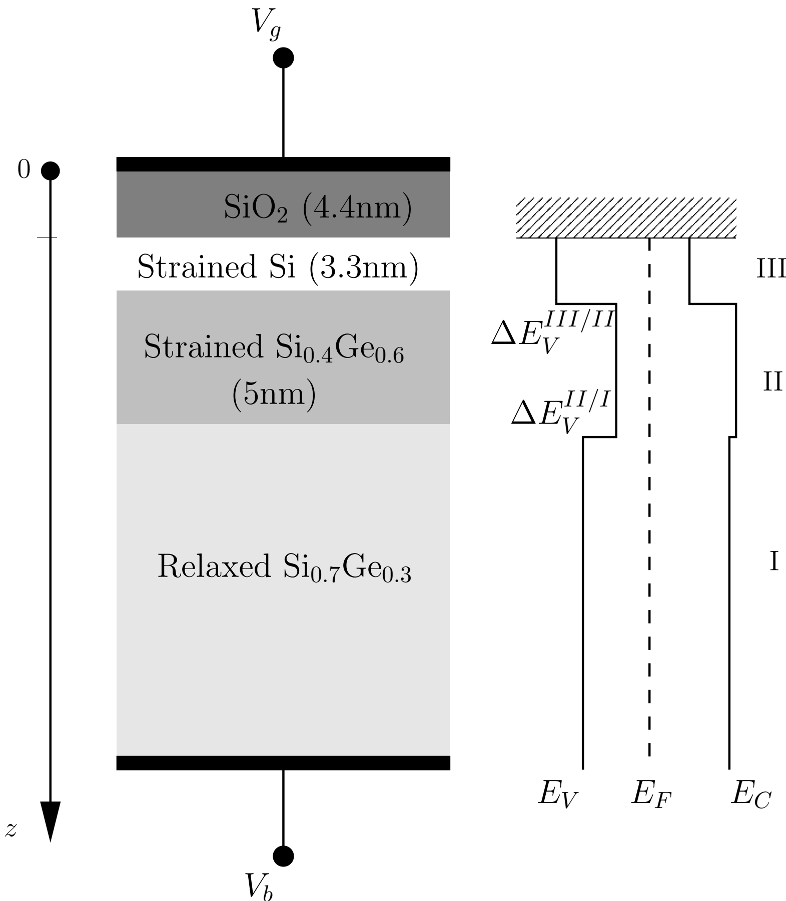
- Schrödinger/Poisson Solver for Strained Si and SiGe
- Density Gradient Model
- Extraction of the heterojunction valence band offsets needed for TCAD simulators
- Conclusion and Outlook

Motivation

multi stacked strained structure



Changes in the band structure and small thickness of the strained layers

$\Longrightarrow$ **Size Quantization**

Solution: Schrödinger equation (SE) with a full band description using the $\mathbf{k} \cdot \mathbf{p}$-method

For TCAD use, directly solving the SE is too CPU intensive.

$\Longrightarrow$ **Density Gradient Method** (DGM)

Problem: unknown model parameters e. g. effective band offsets.

Effective band offsets can be determined by:

- **Measurement:** The effective band offsets can be extracted by inverse modeling of CV measurements based on the DGM [1].

  $\Longrightarrow$ Uncertainty due to incomplete knowledge of the investigated devices

- **Simulation:** Based on the self-consistent solution of the SE and Poisson equations, the effective band offsets can be extracted and the errors of the DGM approximation can be investigated.

[1] C. Ni Chleirigh et al., "Extraction of band offsets in Strained Si/Strained SiGe on relaxed SiGe dual-channel enhanced mobility structures" to be presented at *SiGe Materials, Processing and Devices Symposium*, Hawai, 2004.

Schrödinger/Poisson Solver for Strained Si and SiGe

6×6 $\mathbf{k} \cdot \mathbf{p}$ SE for holes:

$$\left[\widehat{\mathbf{H}}\left(\mathbf{k}, k_z = -i\frac{\partial}{\partial z}\right) + \widehat{\mathbf{I}} \cdot eV(z)\right] \mathbf{F}_{\mathbf{k}}^n(z) \;=\; E_n(\mathbf{k})\mathbf{F}_{\mathbf{k}}^n(z)$$

with $\mathbf{k} = (k_x, k_y)$, $\widehat{\mathbf{H}} = \widehat{\mathbf{H}}_{\mathbf{kp}} + \widehat{\mathbf{H}}_{so} + \widehat{\mathbf{H}}_{str}$ and

$$V(z) \;=\; \Psi(z) \;+\; \Delta E_v^{\mathrm{av}}/e,$$

ΔE_v^{av} [2]: "natural" valance band offset step of the Si/ SiGe heterostructure.

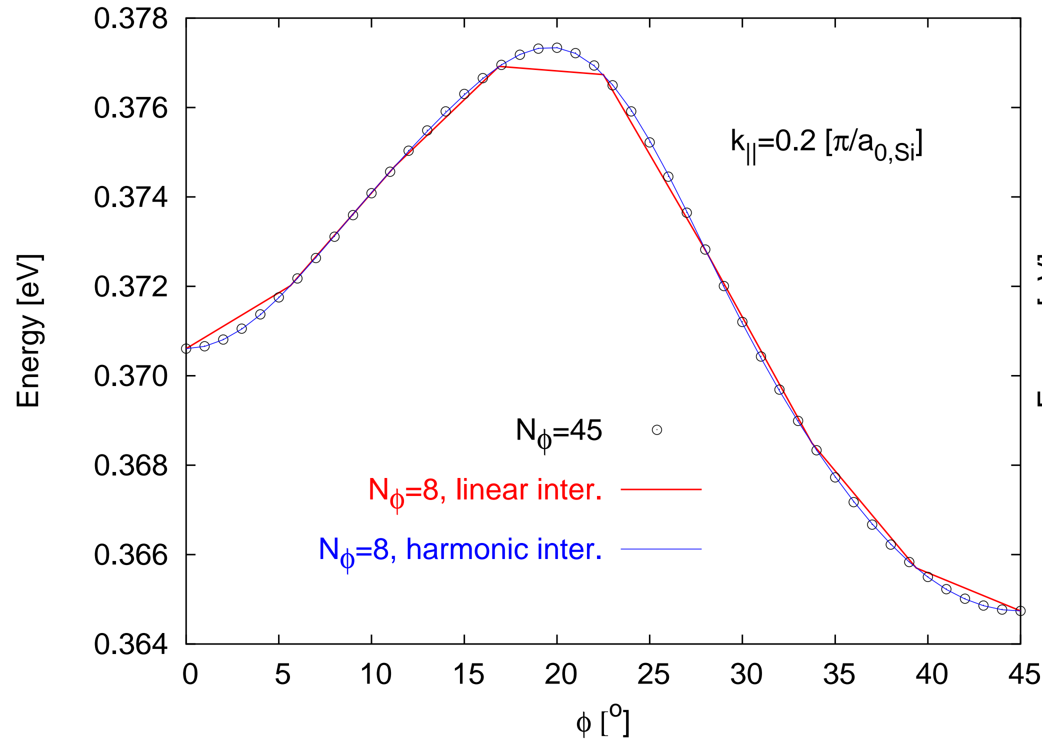
The quantum-mechanical charge density:

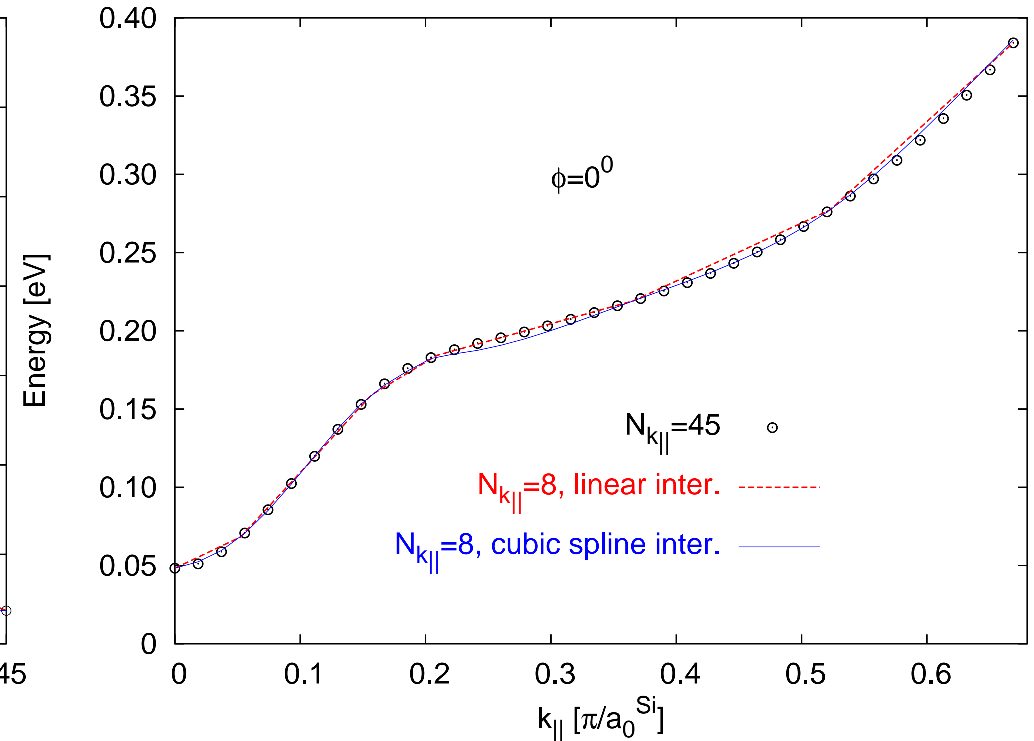
$$p^{\mathrm{qm}}(z) \;=\; \sum_n \frac{1}{(2\pi)^2} \int |F_{\mathbf{k}}^n|^2 f\left(E_n(\mathbf{k}) + E_F\right) \mathrm{d}^2 k \;, \qquad (1)$$

In contrast to *nextnano*^{3}, a modified discretization scheme for the two-dimensional $\mathbf{k}$ space is used in order to reduce the computation time and to calculate (1) with high accuracy. Moreover, the CV characteristics for mobility and band-offset extraction are determined by 1st order perturbation theory. $\Longrightarrow$ About 30 times less CPU intensive than *nextnano*.

[2] C. G. van de Wall Phys. Rev. B, vol. 35, no. 15, pp. 8154–8165, 1987

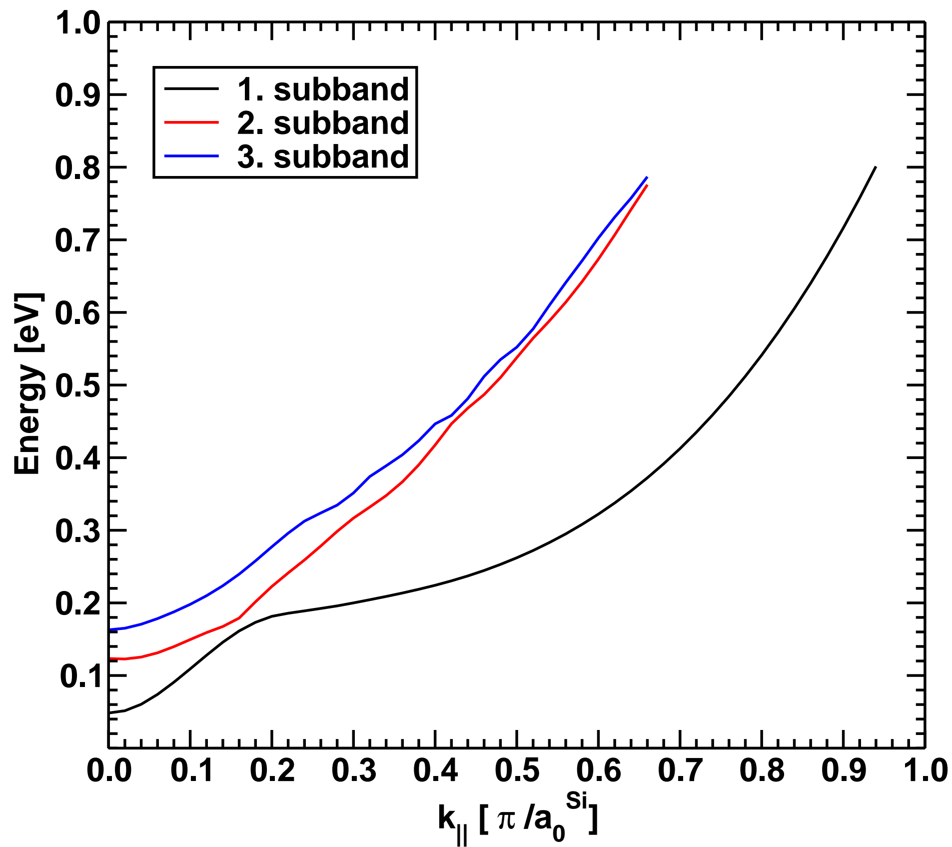
New interpolation method and grid

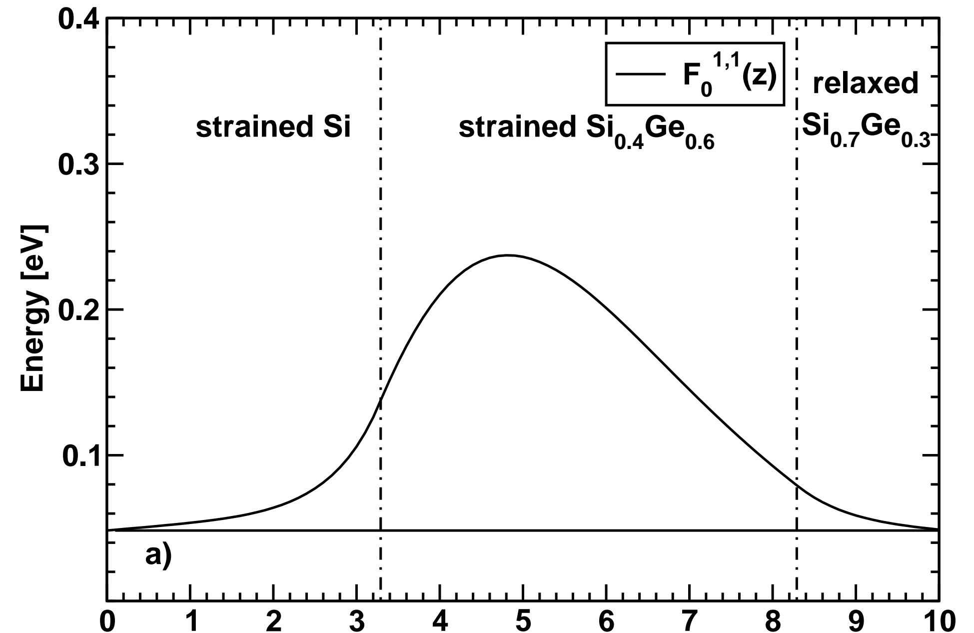




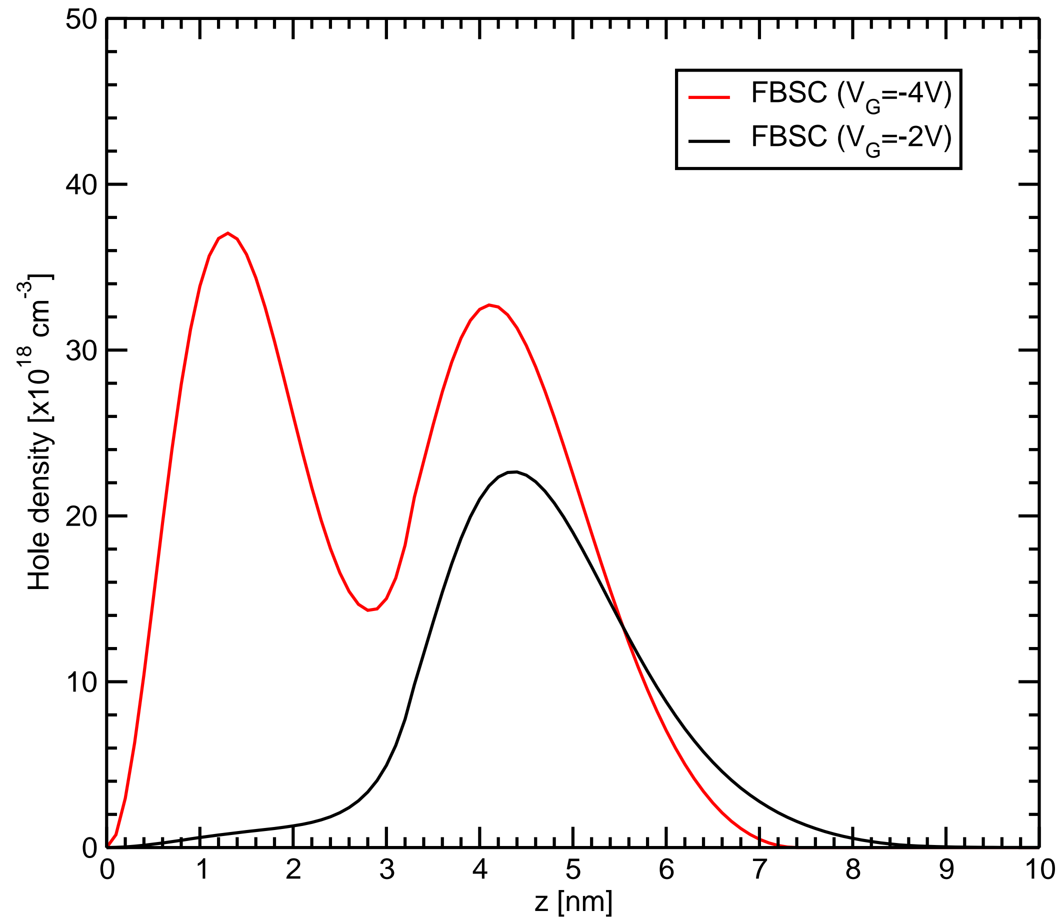
$\Longrightarrow$ CPU-time gain = 25-30

Band structure of first three subbands ($N_D = 5 \times 10^{17}$ cm^{-3}, $V_G = -2.5$V, $\phi = 0^o$) and the wave function of the first energy level.





Hole density at room temperature for two gate biases evaluated by SE



Density Gradient Model

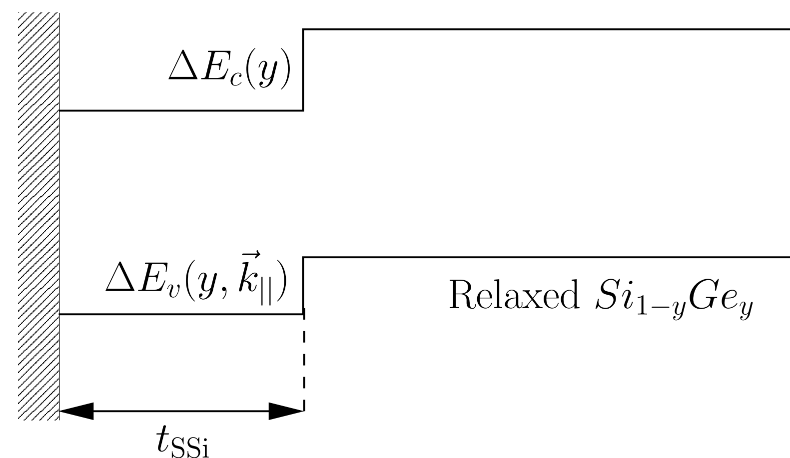
Approximate quantum correction by the density gradient model (DGM):

$$p^{\mathrm{dg}}(z) \; = \; N_v \exp\left(\frac{E_v + \Phi_m + \Lambda - E_F}{k_B T}\right) .$$

Here, $\Phi_m = (3/2) k_B T \log(m^*)$ and Λ is obtained by solving a differential equation:

$$\Lambda = \frac{\hbar^2 \gamma}{12 m}\left\{\nabla \cdot \nabla \frac{\bar{\Phi} - E_F}{k_B T} + \frac{1}{2}\left(\nabla \frac{\bar{\Phi} - E_F}{k_B T}\right)^2\right\}, \quad \text{with } \bar{\Phi} = E_v + \Phi_m + \Lambda$$

What is new in strained material compared to relaxed material?



Electrons:

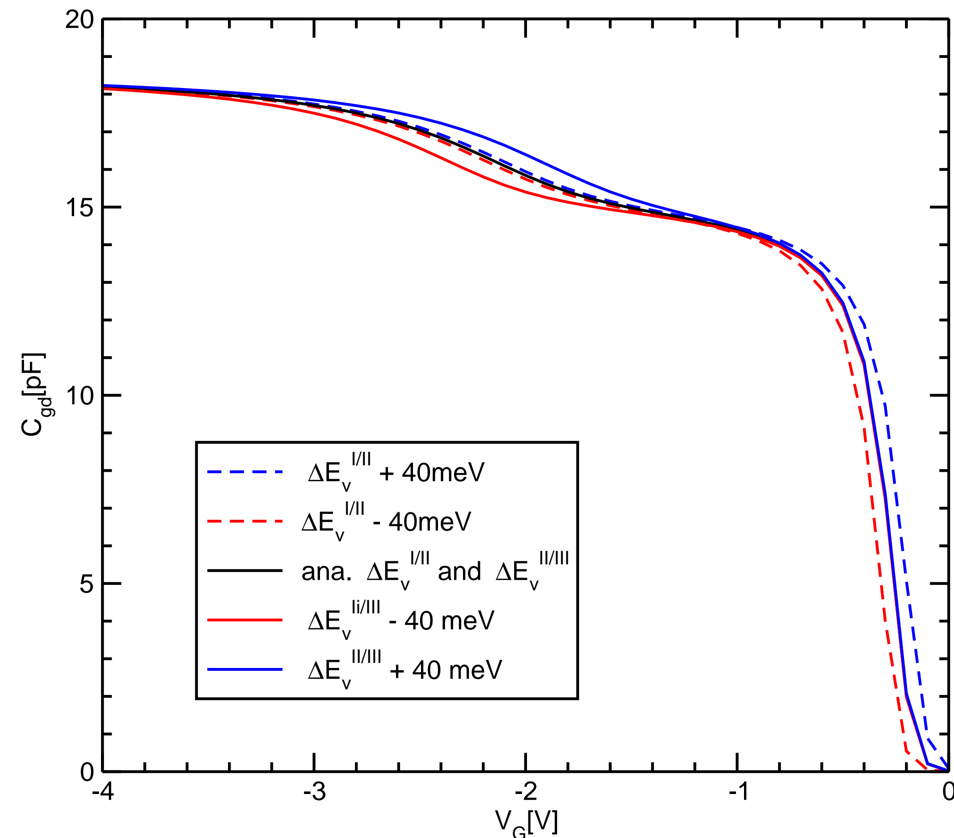
$\Delta E_c(y)$ known from literature.

Holes:

$\Delta E_v(y, \vec{k}_{||})$ depends on $\vec{k}_{||}$

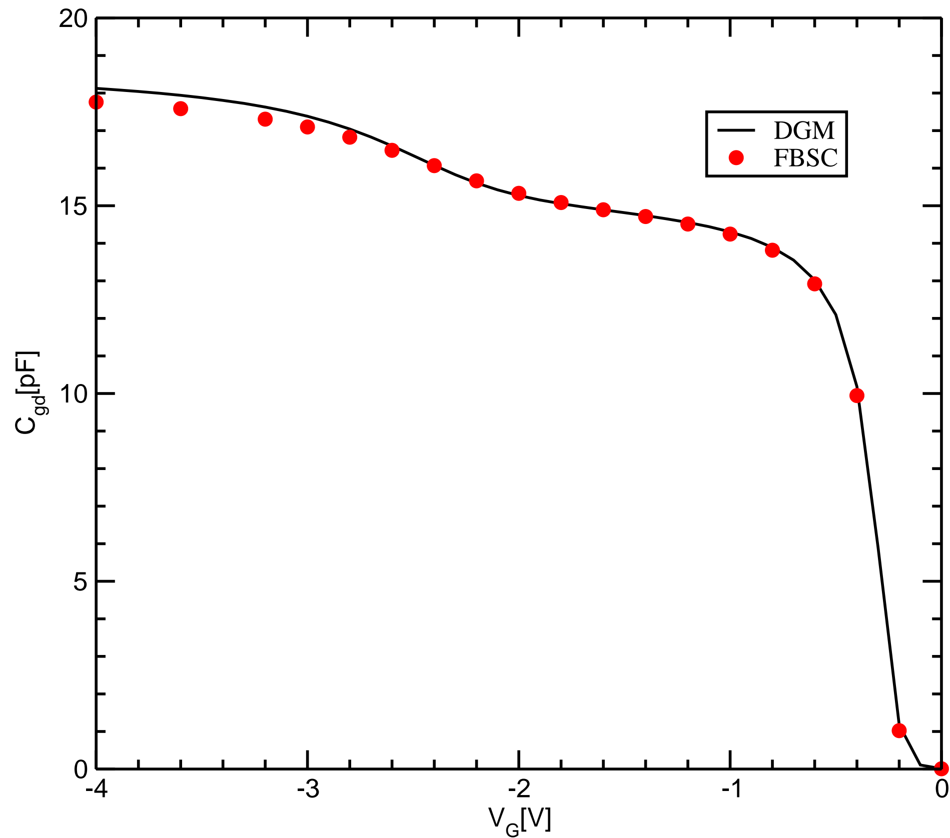
but $\Delta \bar{E}_v(y)$ independent from $\vec{k}_{||}$ required for TCAD (effective valence band offsets)

Extraction of the band offsets for TCAD

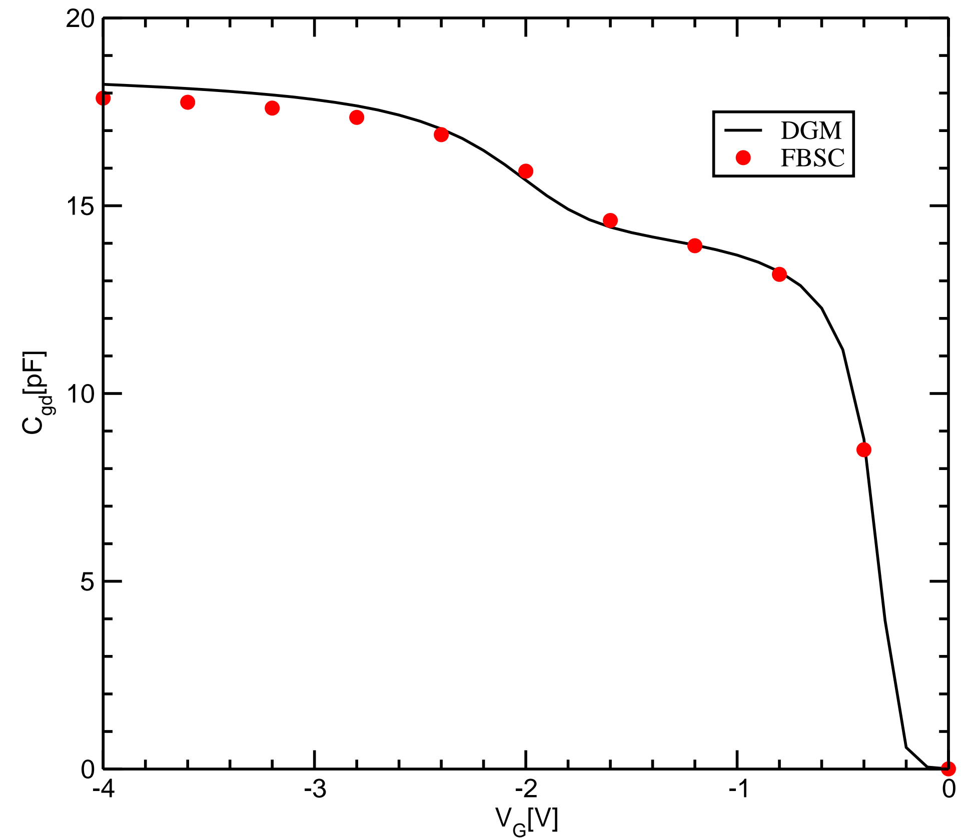


- Based on the CV data calculated by SE, the valance band offsets have been extracted by matching the CV data calculated by DGM.
- The conduction band offsets are fixed during the fitting procedure.
- Note that in this version the effective mass of Si for DGM was used because no values are available for strained Si and strained SiGe.

Gate capacitance with different thickness of strained Si region ($T = 300$ K)



$t_{SSi} = 3.3$ [nm]



$t_{SSi} = 4.0$ [nm]

Conclusion and Outlook

- Conclusions
  - Efficient evaluation of low frequency CV characteristic for multi stacked strained Si structures with a complete description of the valance band structure is now possible.
  - Accurate calculation of CV-characteristics for strained Si/SiGe dual channel pMOSFETs based on Density Gradient Method with the corresponding extracted valance band offsets.
- Outlook
  - Improvement of the state of art Density Gradient Model for holes in strained Si and strained $Si_{1-x}Ge_x$ based on our SE/PE solver.
  - Extraction of the heterojunction valence band offsets and other parameters for wide range of Ge contents.
  - Verification of the extracted results by comparison with measured CV-data.