Fast Methods for Full-Band Mobility Calculation

Z. Stanojević, L. Filipović, O. Baumgartner, and H. Kosina

Institute for Microelectronics, TU Wien, Gußhausstraße 27–29/E360, 1040 Wien, Austria

e-mail: {stanojevic|baumgartner|lidijafilipovic|kosina}@iue.tuwien.ac.at

Introduction and Motivation

Accurate band structure modeling is an essential ingredient in mobility modeling for any kind of semiconductor device or channel. This is particularly true for holes as the valence band of the most commonly used semiconductor materials is not even close to being parabolic. Instead, valence bands exhibit warped structures that simply cannot be approximated with parabolic valleys. To make matters worse, nanostructured channels can have large quantization energies resulting in complex, highly orientation-dependent kinetic behavior of both holes and electrons [1].

In this work, we present an accurate and computationally efficient method for calculating channel low-field mobilities a numeric band structure from a $\mathbf{k}\cdot\mathbf{p}$ model.

Modeling and Implementation

The band structure is modeled using a $\mathbf{k}\cdot\mathbf{p}$-Hamiltonian. The Hamiltonian is discretized and the subband structure extracted using the Vienna Schrödinger-Poisson (VSP) simulation framework [2].

In our model we assume a small deviation of the distribution function $f^0 \mapsto f^0 + f^1$ due to a small electric field along the channel. Rather than making any assumptions about f^1 we compute it directly by numerically solving the Boltzmann transport equation in the low-field approximation

$$\sum_{n',\mathbf{k}'} S_{n,n'}(\mathbf{k},\mathbf{k}')\big[f_n^1(\mathbf{k}) - f_{n'}^1(\mathbf{k}')\big] =$$

$$-\frac{1}{\hbar}\mathbf{F}\cdot\boldsymbol{\nabla}_{\mathbf{k}}f_n(\mathbf{k}) \approx -\mathbf{F}\cdot\mathbf{v}_n(\mathbf{k})\frac{\mathrm{d}f^0}{\mathrm{d}E},$$

on a $\mathbf{k}$-grid. This also ensures accurate treatment of anisotropic scattering processes such as Coulomb or roughness scattering.

The couplings between states due to scattering are determined by contour-integration of the subband structure. The resulting coupling matrix is sparse and the implemented algorithm exploits the sparsity to reduce computation time and memory consumption.

For each non-zero coupling, transition rates are calculated as derived from Fermi's golden rule. Apart from phonon and impurity scattering we also adapted our recently developed surface roughness scattering (SRS) model for non-planar structures [3], [4] to full-band calculations. The key point is the use of *form functions* analogous to the form factors in the Prange-Nee model for planar surfaces. The planar transition rate

$$S_{n,n'}(\mathbf{k},\mathbf{k}') = \frac{\pi}{\hbar}\frac{C(\mathbf{q})}{A}|F_{n,n';\mathbf{k},\mathbf{k}'}|^2$$

is replaced with

$$S_{n,n'}(\mathbf{k},\mathbf{k}') = \frac{1}{2\hbar L}\int_{\mathbb{R}}|F_{n,n';\mathbf{k},\mathbf{k}'}(q_\perp)|^2 C(\mathbf{q})\mathrm{d}q_\perp,$$

where $F_{n,n';\mathbf{k},\mathbf{k}'}(q_\perp)$ are the Fourier transforms of the form functions and $C(\mathbf{q})$ the roughness power spectrum.

Results and Conclusions

To demonstrate the developed methods and the insights they provide, we show example calculations of a circular nanowire (Fig. 1) and of a double-gate UTB channel (Fig. 4). In both cases the valence band is of primary interest due to its warped, non-parabolic structure. A qualitative difference between phonon scattering and SRS can be observed in both cases (Figs. 2 and 5) resulting in a complex $\mathbf{k}$-space distribution of the low field current (Figs. 3 and 6). It is important to note that both examples are run using the same, dimension-independent code. This ensures the consistency of results and allows cross-calibration of parameters between planar and non-planar channels.

We developed a number of methods targeted at fast full-band mobility calculation of device channels, including: subband structure calculation, determination of couplings in $\mathbf{k}$-space, and evaluation of the transition rates based on our recent modeling efforts of SRS. The entire workflow is implemented within the Vienna Schrödinger-Poisson (VSP) simulation framework. Every step in the process is parallelized with close-to-linear scalability. The resulting performance boost brings full-band mobility modeling one significant step closer to mainstream TCAD device simulation.

Acknowledgment

References

[1] N. Neophytou *et al.*, Solid-State Electronics **70**, 81 (2012).
[2] O. Baumgartner *et al.*, J. Comput. Electron. (2013).
[3] Z. Stanojevic *et al.*, Intl. Conf. on Simulation of Semiconductor Processes and Devices (2013), pp. 352–355.
[4] Z. Stanojevic *et al.*, Intl. Electron Device Meeting (2013).

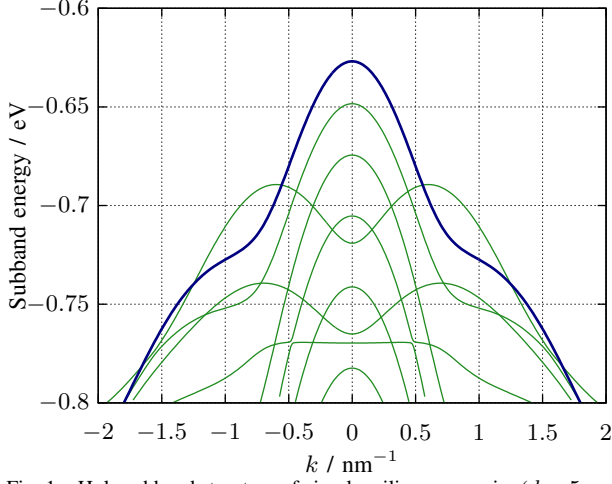Fig. 1. Hole subband structure of circular silicon nanowire ($d = 5\,\mathrm{nm}$) with a $\langle 110 \rangle$ axis; ensuring correct continuation of each subband, the subbands can be seen to cross each other at several points as highlighted in the first subband.
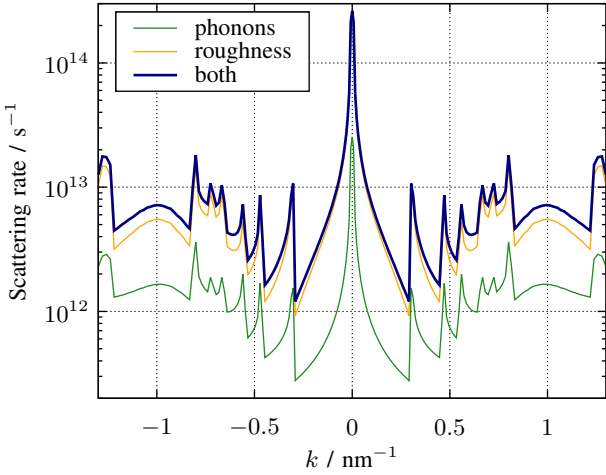

Fig. 2. k-resolved scattering rates for the lowest hole subband; singularities in the rates typical of a 1DEG can be seen. The rates for phonon scattering and SRS deviate strongly from each other.
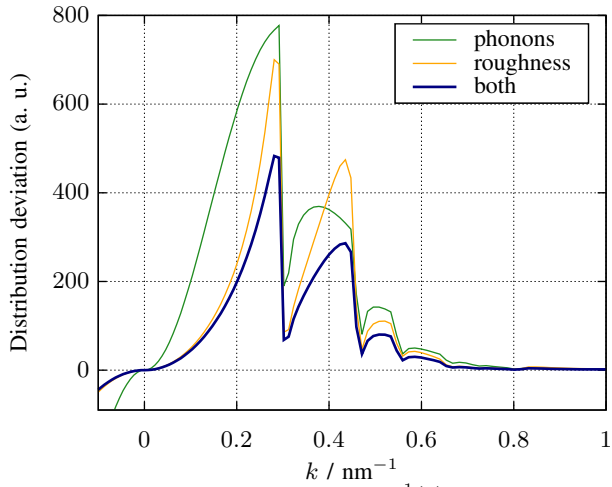

Fig. 3. Field-induced distribution deviation $f_n^1(k)$ (shown for the lowest subband) under different scattering processes; the anisotropic nature of SRS repels the carriers from the zone center; the functions could not be described analytically justifying their numerical calculation.
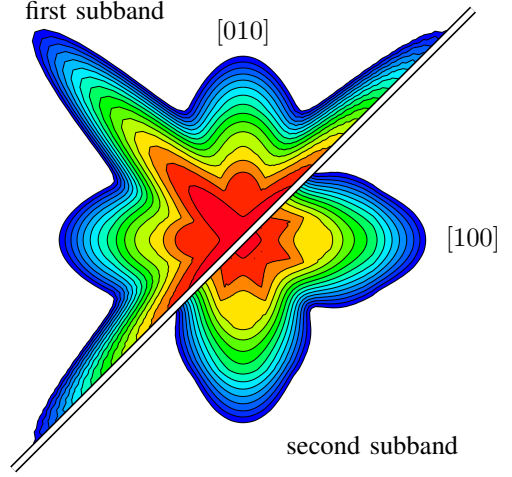

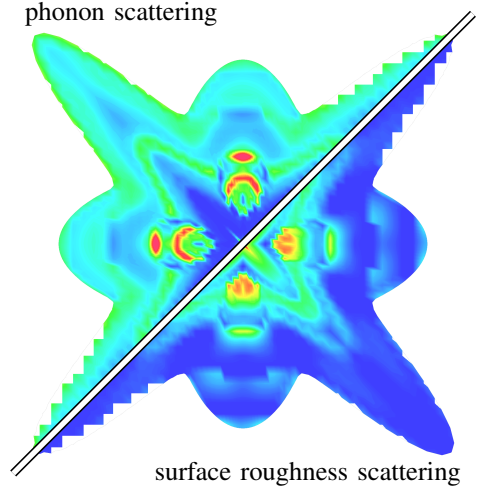Fig. 4. The top two hole subbands of a $5\,\mathrm{nm}$ thick UTB with [001] surfaces

Fig. 5. k-resolved phonon and surface roughness scattering (SRS) rates in the first subband; SRS prefers small deflections and is thus more pronounced near the Γ-point, whereas phonon scattering becomes stronger for large k-values.
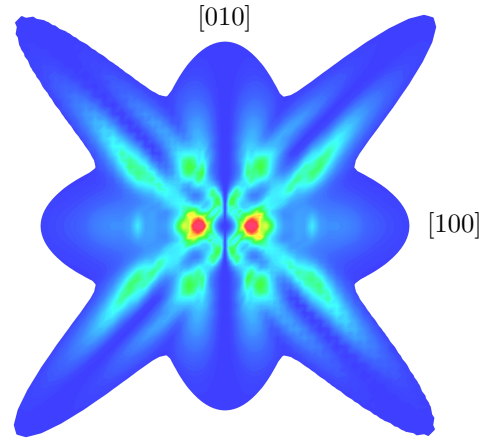

Fig. 6. k-resolved distribution of the low-field current in all subbands for an electric field applied in [100] direction.