Spherical Harmonics Expansion of the Conduction Band for Deterministic Simulation of SiGe HBTs with Full Band Effects

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***Abstract*— A SiGe HBT is simulated using a deterministic Boltzmann equation solver with full band effects. An anisotropic band structure fitted to full band for high energies significantly improves the simulation of SiGe HBTs with a spherical harmonics expansion solver, especially when it comes to breakdown voltages. This makes it a more efficient alternative to stochastic Monte Carlo simulation.**

I. Introduction

The scaling of devices causes the drift-diffusion and the hydrodynamic model to fail as transport becomes quasi-ballistic [1]. Therefore the Boltzmann transport equation (BTE) must be solved with fewer simplifications. This is often accomplished by stochastic Monte Carlo simulation with a number of disadvantages including inefficiency when evaluating small currents and rare events like impact ionization. A spherical harmonic expansion (SHE) of the distribution function allows a direct solution of the BTE, but is restricted to either first order expansion [2], which is not sufficient for nanoscale devices [3], or a simplified band structure [4]. In this paper we present a band structure for a SHE solver [5] that captures full band effects and can be used with arbitrary order SHE. This enables accurate modeling of high energy effects such as impact ionization which is critical for evaluating e.g. the multiplication factor of a SiGe HBT.

II. Theory

The SHE solver for higher order expansion requires a bijective dispersion relation with respect to the modulus of the wave vector $k(\varepsilon,\theta,\phi)$ [3]. Consequently, full band structure can only be utilized up to an energy of 0.12eV for the conduction band in Si. An approximation is necessary above this value. The Modena model [6] previously adopted is inaccurate at higher energies when compared with full band Monte Carlo (MC).

The adoption of a three-valley model makes possible the inclusion of anisotropic effects which become more important with higher SiGe content in the base region of a SiGe HBT. In pure silicon all three valleys are identical except for rotation. As a result only one valley needs to be described, whereas others can be included by rotation. Ge-content and biaxial strain is taken into account with an offset in the band gap of $\varepsilon_{\text{shift}} = 0.6305\text{eV} \cdot X_{\text{Ge}}$ of the valley in transport direction. X_{Ge} is the germanium mole fraction.

To approximate the valley we use real spherical harmonics (SH) expansion of the Herring-Vogt transformed [7] inverse dispersion relation similar to the approximation done in [8] for the valence band:

$$k(\varepsilon,\theta,\phi) = \sum_{l,m\geq 0} k_l^m(\varepsilon) P_l^m(\cos\theta)\cos(m\phi) \tag{1}$$

with ε being the energy, θ the inclination, ϕ the azimuth, $P_l^m(\cos\theta)$ the associated Legendre function and $k_l^m(\varepsilon)$ the fitting quantity. By positioning the origin in the minimum of a valley and orientating the polar axis with the $\langle 100\rangle$ axis of the crystal structure, we can assume a large share of the SH coefficients to be zero due to symmetries. This leaves us with only positive m-values which are a multiple of four and even l-values.

For the first 120meV, coefficients are calculated through direct SHE of the conduction band. The results serve as a starting value for the optimization using the Levenberg-Marquardt algorithm [9] at higher energies. A full-scale simulation for every iteration in the optimization would lead to prohibitive CPU time. Instead, the quadratic error of the moments

$$V_0(\varepsilon) := \frac{1}{(2\pi)^3}\int_{\text{BZ}} \delta\left(\varepsilon - \varepsilon(\mathbf{k})\right) d\mathbf{k} \tag{2}$$

and for $n = 1...5$

$$V_n(\varepsilon) := \frac{\frac{1}{(2\pi)^3}\int_{\text{BZ}} |\mathbf{v}(\mathbf{k})|^n \delta\left(\varepsilon - \varepsilon(\mathbf{k})\right) d\mathbf{k}}{V_0(\varepsilon)} \tag{3}$$

in comparison with full band data serves as the objective function. $\mathbf{v}$ denotes the group velocity and $\int_{\text{BZ}} d\mathbf{k}$ the integral over the Brillouin zone. Note that V_0 is proportional to the average density of states. These moments have been selected as the accuracy of the deterministic solver is strongly correlated with good agreement of the moments with fullband structure. It turns out that the most significant trade-off occurs between 0th order moment and higher order moments. In order to limit inaccuracies in the density of states, V_0 receives higher weight

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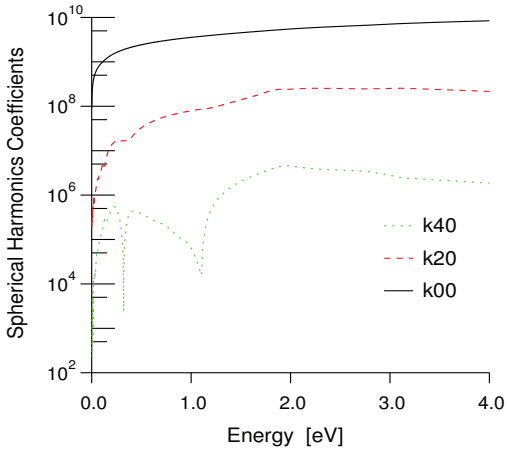

Fig. 1. k_{lm} coefficients over energy with normalized spherical harmonics (arbitrary unit)

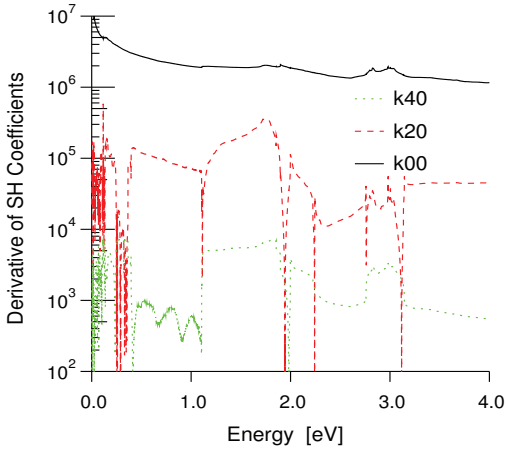

Fig. 2. Partial derivative of the k_{lm} coefficients with respect to energy using normalized spherical harmonics calculated by finite difference approximation (arbitrary unit)

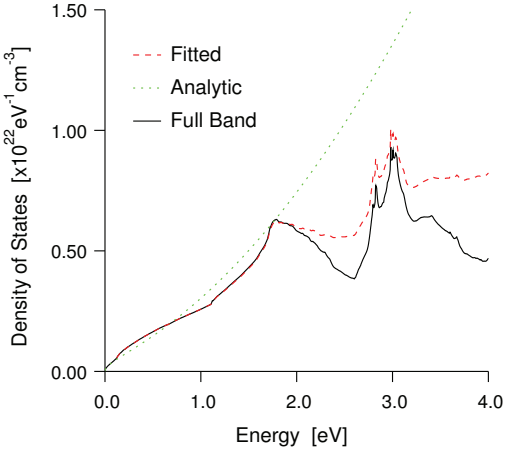

Fig. 3. Fitting target – average density of states using the full band fit results, analytical Modena band structure and full band Monte Carlo

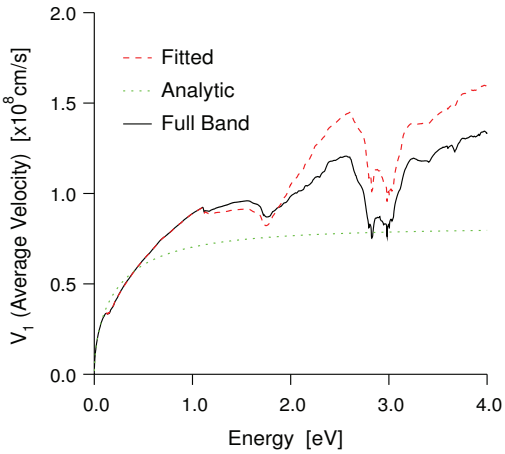

Fig. 4. Fitting target – first moment V_1

in the target function. The coefficients k_{lm} are calculated with a discretization of 1meV based on the optimization result of the previous energy level and on the analytical calculation of the coefficients to exactly match the density of states.

A positive derivative over all angles and energy steps can be enforced directly in the target function through introducing an additional term as a penalty for low derivatives of the inverse dispersion relation for all θ and ϕ. This also prevents problems resulting from an insufficient grid, if derivatives change rapidly with angle.

Holes in device simulation are considered using a simple drift-diffusion model.

III. Results

Remarkable gains are only visible when the dispersion relation is expanded up to 4th order. Thus all graphs shown in this paper use a 4th order SH-expanded band structure.

Figures 1 and 2 show convergence of the SH coefficients and their derivatives with increased l-value. The SH coefficients in these figures have been normed so that equal difference in coefficients leads to an equal maximum difference of the SHE. Rapid decay in values of approximately two orders of magnitude is observed, therefore expanding up to 4th order is apparently sufficient.

Density of states (figure 3) and the first moment (figure 4, average velocity) cannot fit perfectly at high energies since only positive $dk/d\varepsilon$ is allowed, but up to two eV good agreement is achieved. In modern devices impact ionization mostly occurs between 1.1eV and 2eV due to low operating voltages. Hence we can expect realistic results. Nevertheless, the resulting bulk distribution function is significantly improved for all relevant electric fields even at higher energies (figure 5).

The direct dependence on the high energy distribution function translates into accurate calculation of impact ionization because it matches the full band values almost exactly (figure 6).

We simulate an example SiGe HBT with a 20% Ge biaxially strained base and a 100GHz cutoff frequency. The doping profile is displayed in figure 7.

Calculated cutoff frequencies match full band much better

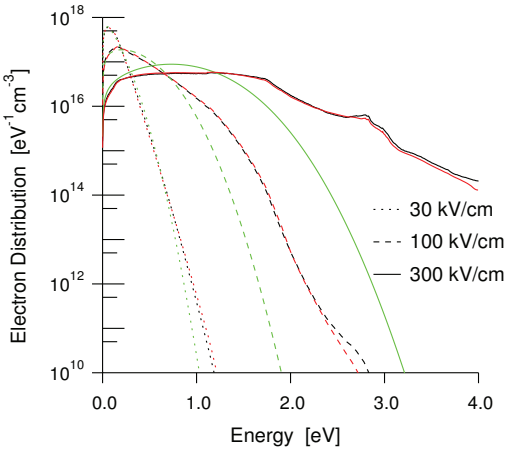

Fig. 5. Bulk distribution function in ⟨100⟩ direction for different electric fields without impurity scattering, colors are matched to band structures as in figure 4

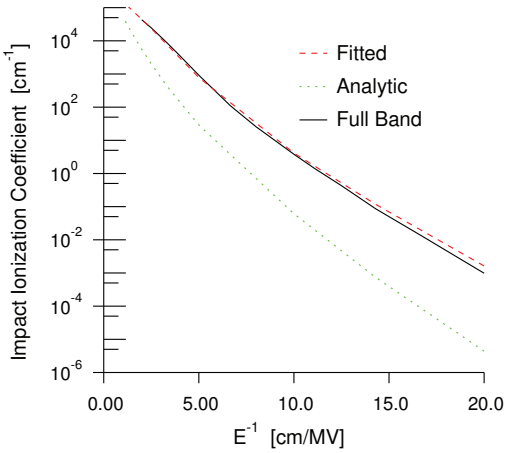

Fig. 6. Impact ionization coefficient over inverse electric field in bulk simulation

than simulation results with Modena band structure (figure 8). Impact ionization does not play a significant role here, which suggests that accurate band structure modeling is also important for lower operating voltages.

Impact ionization rates fit well also in devices (figure 9).

Figure 10 highlights the enhanced distribution function, on which the impact ionization relies. This leads to an accurate evaluation of multiplication factors (figure 11) and consequently breakdown voltages.

The simulation of cutoff frequencies, as defined by Gummel [10], is particularly time intensive with Monte Carlo because we have to calculate the partial derivative of charge with respect to collector current with finite differences. The SHE solver provides results about 300 times faster with the same accuracy. The SHE error is defined by comparison with a simulation with a much higher order of SHE and a finer energy discretization, while the MC error is defined as twice the standard deviation.

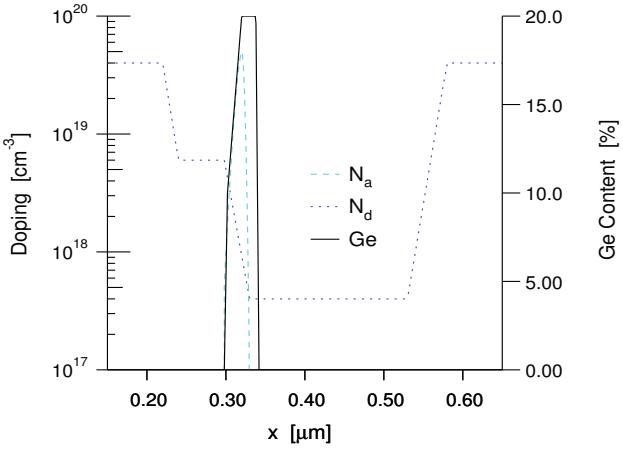

Fig. 7. Doping and germanium profile of a $f_t \approx$ 100GHz device

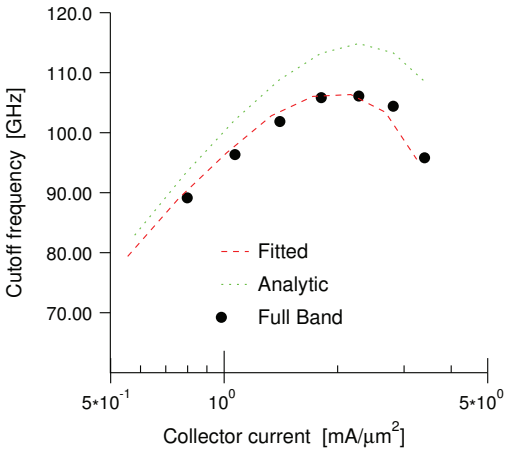

Fig. 8. Cutoff frequency f_t at V_{BE} = 0.7V

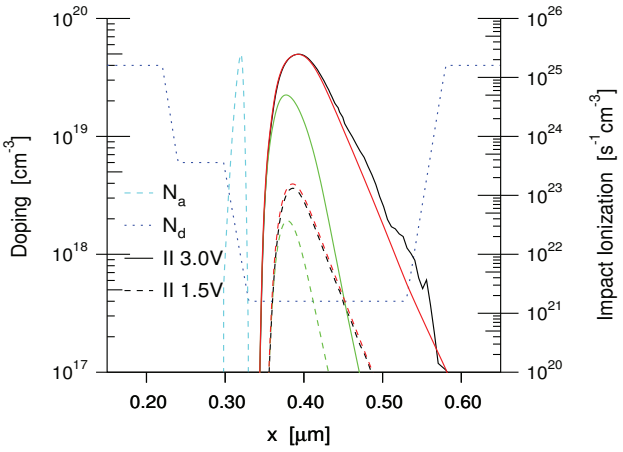

Fig. 9. Impact ionization over the device at V_{BE} = 0.8V at different V_{CE} values, colors are matched to band structures as in previous figures

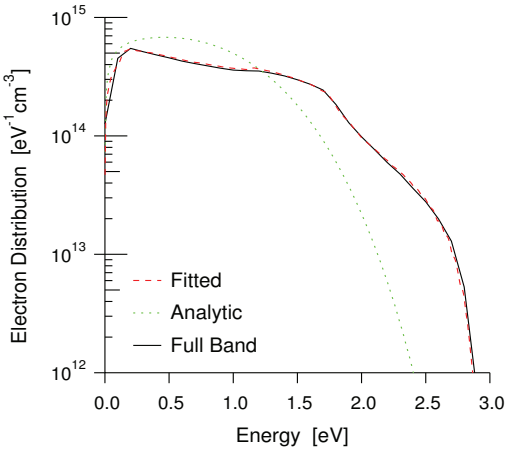

Fig. 10. Electron distribution function at the location with highest impact ionization, V_{BE} = 0.7V and V_{CE} = 3V

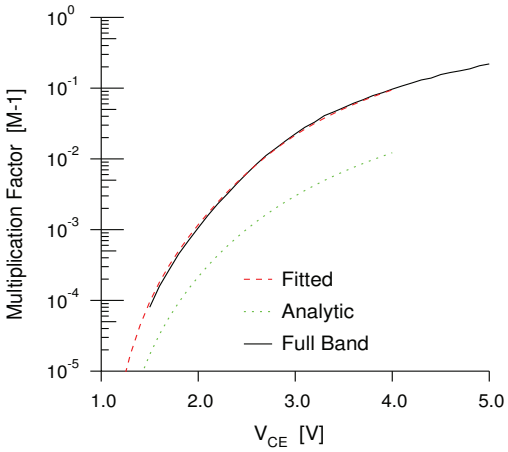

Fig. 11. Multiplication factor $M-1$ for the 100GHz device at $V_{BE} = 0.7$V

IV. Conclusion

Results demonstrate that SHE is a viable alternative to MC for predictive simulation of SiGe HBTs. The approximation of the full band structure presented in this paper produces much better results than the previously used Modena band structure. This can be a very helpful tool in exploring the limits of the SiGe HBT technology.

Acknowledgment

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