A Full-Band Spherical Harmonics Expansion of the Valence Bands up to High Energies

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***Abstract*— The valence bands of silicon can be expanded exactly by spherical harmonics only up to the energy, where the bands reach the surface of the Brillouin zone (BZ). For higher energies an approximation is required. Therefore an anisotropic extension of the band structure is presented which is determined by matching the density of states (DOS) and moments of the inverse group velocity of the exact full-band (FB) structure. The Boltzmann equation (BE) based on the exact FB at low energies and the approximation at high energies is solved by the spherical harmonic expansion (SHE) method for bulk silicon including impact ionization. The results are compared to Monte Carlo (MC) data based on the exact FB structure.**

I. Introduction

In Ref. [1] a SHE of the valence band structure has been presented. This expansion is only possible as long as the energy depends in a monotonic way on the wave vector. For heavy holes in unstrained silicon this is the case up to about 1.27eV limiting the usefulness of this approach. We present an approximation with which this approach can be extended to higher energies. In contrast to previous work (e.g., [2]), our approach is anisotropic and the DOS and the group velocity are consistent with the band structure, which is a prerequisite for a stable discretization of the BE in devices [3].

In section 2, the theory for the anisotropic extension of the valence band is described. The DOS and moments of the inverse group velocity are matched to those of the exact FB structure [4]. With the valence bands extended up to high energies meaningful hot hole simulations are possible, and the BE is solved at high electric fields by the SHE method for bulk silicon including impact ionization. The results, which are shown in section 3, are compared to MC data based on the exact FB structure [5].

II. Theory

The SHE of the distribution function on equienergy surfaces has many advantages over an expansion with respect to the modulus of the wave vector [3]. The BE is therefore projected onto SHs for constant energies. This requires the mapping of the spherical coordinates of the $\vec{k}$ space (k, θ, ϕ) onto an energy space (ε, θ, ϕ), where the angles are the same in both spaces. This is only possible as long as the mapping is unique in both directions [1]. In the case of the FB structure for heavy holes in unstrained Si, this is possible up to 1.27eV (light holes: 1.31eV, split off: 7.09eV). For higher energies, the bands are constructed in such a way that, on the one hand, the dispersion relation $k^\nu(\varepsilon,\theta,\phi)$ of band ν depends monotonic on ε for all angles (θ, ϕ), and on the other hand, the moments

$$V_n(\varepsilon) \equiv \sum_\nu \int_{\mathrm{BZ}} \frac{1}{|\vec{v}^\nu(\vec{k})|^n} \delta(\varepsilon - \varepsilon^\nu(\vec{k}))d\vec{k} \tag{1}$$

are reproduced as good as possible. $\vec{v}^\nu(\vec{k})$ is the group velocity in $\vec{k}$ space, n an integer number and the integral is taken on the equienergy surface $\varepsilon^\nu(\vec{k}) = \varepsilon$ within the first BZ. With the methods presented in Ref. [5] the moments V_n are calculated by numerical integration over the first BZ of the FB structure [4]. However for evaluating the integral V_n in spherical coordinates $(\varepsilon,\theta,\phi)$, k and its derivatives with respect to energy and angles are required for all (θ,ϕ). The construction for k at high energies is based on a recursive calculation of $k^\nu(\varepsilon,\theta,\phi)$ from its value $k^\nu(\varepsilon-\delta\varepsilon,\theta,\phi)$ at the energy $\varepsilon-\delta\varepsilon$, where $\delta\varepsilon$ denotes the energy spacing. The initial value of k is given by the value at the highest energy for which the exact FB can be still expanded. The approximative SHE of $k^\nu(\varepsilon,\theta,\phi)$ is obtained by adding a few low order SH terms to the previous $k^\nu(\varepsilon-\delta\varepsilon,\theta,\phi)$. In addition, the SHE of k contains only even harmonics and has a fourfold symmetry in ϕ due to the symmetry of the band structure [3]. Adding even SHs up to the fourth order to $k^\nu(\varepsilon-\delta\varepsilon,\theta,\phi)$ yields

$$\begin{aligned} k^\nu(\varepsilon,\theta,\phi) = {} & k^\nu(\varepsilon-\delta\varepsilon,\theta,\phi) + \min_{\theta,\phi} k^\nu(\varepsilon-\delta\varepsilon,\theta,\phi) \\ & \times \left[[\gamma_0^\nu(\varepsilon)]^2 + \Gamma^\nu(\varepsilon,\theta,\phi) - \min_{\theta,\phi} \Gamma^\nu(\varepsilon,\theta,\phi) \right] \end{aligned} \tag{2}$$

with

$$\begin{aligned} \Gamma^\nu(\varepsilon,\theta,\phi) = {} & \gamma_1^\nu(\varepsilon)\cos^2\theta + \gamma_2^\nu(\varepsilon)\cos^4\theta \\ & + \gamma_3^\nu(\varepsilon)\sin^4\theta\cos 4\phi \end{aligned} \tag{3}$$

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where $\gamma^{\nu}_{0,1,2,3}$ are fitting parameters. With this ansaltz, obviously $k^{\nu}(\varepsilon,\theta,\phi) \geq k^{\nu}(\varepsilon-\delta\varepsilon,\theta,\phi)$. It means that without any restriction for the fitting parameters, the monotonicity condition of $k^{\nu}(\varepsilon,\theta,\phi)$ is automatically fulfilled for all angles (θ,ϕ). The derivatives of $k^{\nu}(\varepsilon)$ with respect to (w.r.t) the angles can be calculated in a straight forward manner. The derivative of k^{ν} w.r.t energy is determined by a left sided finite difference approximation:

$$\frac{\partial k^{\nu}(\varepsilon,\theta,\phi)}{\partial\varepsilon} = \frac{k^{\nu}(\varepsilon,\theta,\phi) - k^{\nu}(\varepsilon-\delta\varepsilon,\theta,\phi)}{\delta\varepsilon}. \qquad (4)$$

With (2), (4) and the derivatives of $k^{\nu}(\varepsilon)$ w.r.t angles, V_n can be expressed in terms of the fitting parameters and the known k^{ν}, $\vec{v}^{\nu}$ at energy $\varepsilon-\delta\varepsilon$. Matching the V_n to the exact values of the FB structure by the nonlinear least square error Levenberg-Marquardt method [6], [7] yields the set of $\gamma^{\nu}_{0,1,2,3}$ for energy ε. As soon as the fitting parameter set has been obtained for ε, the resultant $k^{\nu}(\varepsilon,\theta,\phi)$ is used as initial value for the dispersion relation of the next energy level $\varepsilon+\delta\varepsilon$. By iteration the fitting parameters are obtained for all energies.

To minimize iteration steps for each energy level, the fitting parameters must be initialized in a proper way. By using small energy steps, the resultant fitting parameters at energy ε can be used as first guess for the optimization of the next energy level $\varepsilon+\delta\varepsilon$. For the energy level at the beginning of the whole optimizing process, all fitting parameters are initialized as zeroes except γ^{ν}_0. With the assumption that the initialized γ^{ν}_0 $(=\gamma_{0,\text{init}})$ are the same for all bands, $\gamma_{0,\text{init}}$ can be found by matching V_0 with its exact value.

The described method allows to extend the SHE of the FB to the high energies required for meaningful hot hole simulations. The BE is solved with a deterministic SHE method based on the phonon system described in Ref. [5] and the impact ionization model of Ref. [8].

III. Results

Up to an energy of 7.09eV the band structure extension is only required for the heavy (HH) and light hole (LH) bands, because the relation between energy and wave vector remains monotonic for the split-off band in this energy range. For energies below 1.2eV, the exact SHE of the HH and LH bands is used. The optimizing process is performed for energies above 1.2eV with an energy step of 1meV. The band index in definition (1) for moments V_n represents HH and LH bands. Fig. 1 - 5 show that V_0 ($\sim$DOS) and V_1-V_5 based on the approximated band structure fit well the exact FB data. The fitting parameters as functions of energy are shown for HH (Fig. 7) and LH band (Fig. 8). It can be seen that $\gamma_0,\gamma_1,\gamma_2 \neq 0$ for both HH and LH bands. This means that the extension of HH and LH bands is anisotropic. Moreover, $|\gamma_3| \ll |\gamma_2|,|\gamma_1|$ implies that the contribution of the harmonic $Y_{4,4}$ ($\sim \sin^4\theta\cos 4\phi$) to the SHEs of the HH and LH bands can be neglected.

The hole drift velocity calculated by SHE for different directions of the electric field is shown together with MC data based on the exact FB in Fig. 9. Good agreement of both methods is obtained and the full anisotropy is reproduced by SHE. In the nonlinear regime, if the applied electric field is rotated by 45^o from $\langle 110\rangle$ to $\langle 100\rangle$ direction, the hole drift velocity increases significantly. The energy distribution function (e.d.f.) is plotted in Fig. 10. The SHE results reproduce accurately the MC results, even for $E = 300$kV/cm. Fig. 11 shows the II coefficient versus inverse electric field. Again the deviation from MC is very small. For $E = 200$kV/cm, it takes six days to obtain the II coefficient with 0.5% error by MC, whereas the CPU time required by SHE is only about eight minutes.

IV. Conclusions

We have developed for the first time an anisotropic method to extend the SHE of the valence bands to high energies and the results agree well with simulations based on the exact FB structure. Since the expansion is exact below 1.2eV, all the important magnetotransport and transport effects in confining fields, which are due to the anisotropic band structure, are described correctly in contrast to previous approaches, which were based on an isotropic approximation of the band structure (e.g., [2]). In addition, our approach avoids the inconsistency of the group velocity and density of states inherent to those schemes.

References

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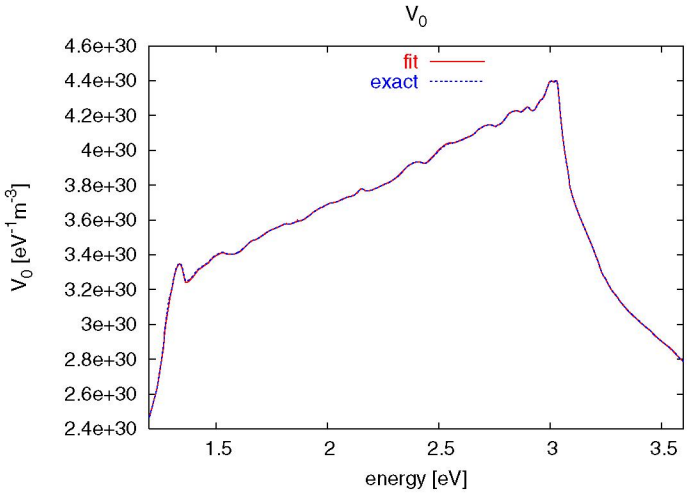

Fig. 1. V_0 contributing by HH and LH bands

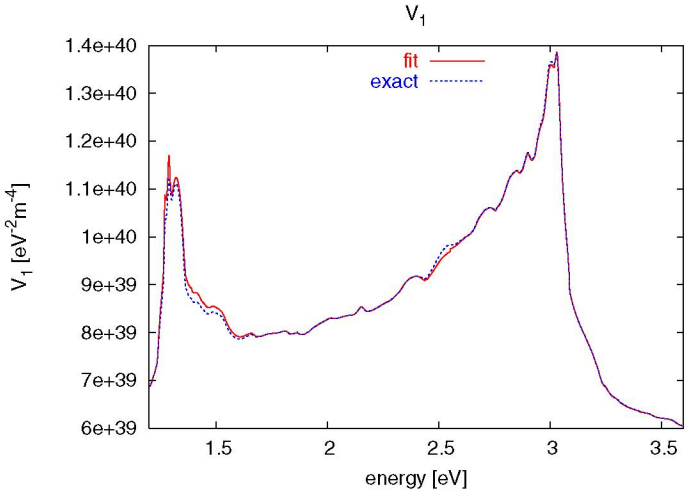

Fig. 2. V_1 contributing by HH and LH bands

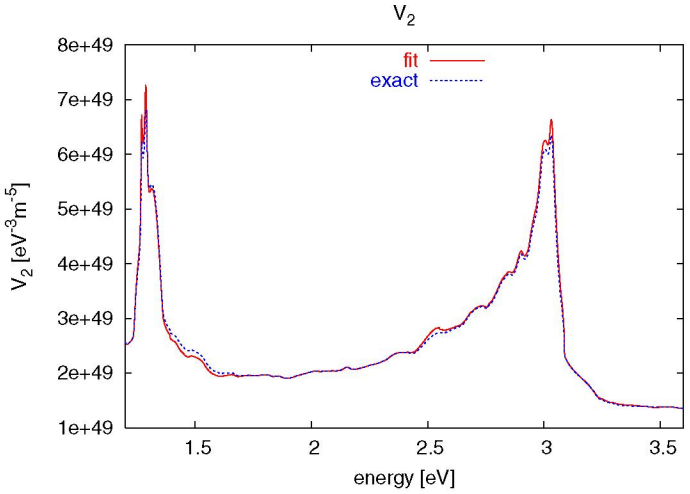

Fig. 3. V_2 contributing by HH and LH bands

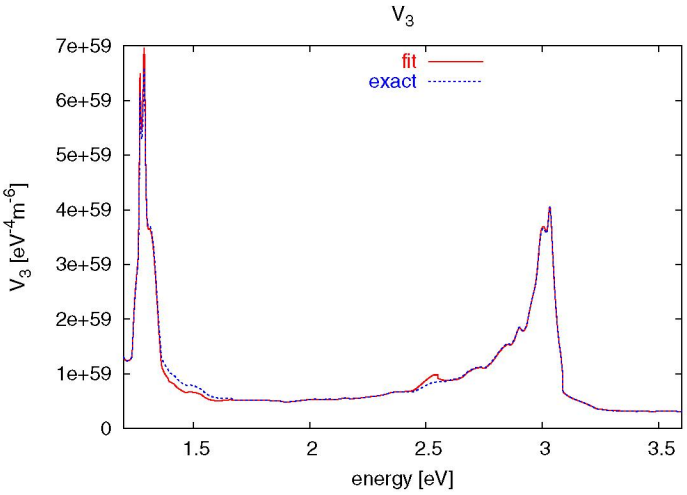

Fig. 4. V_3 contributing by HH and LH bands

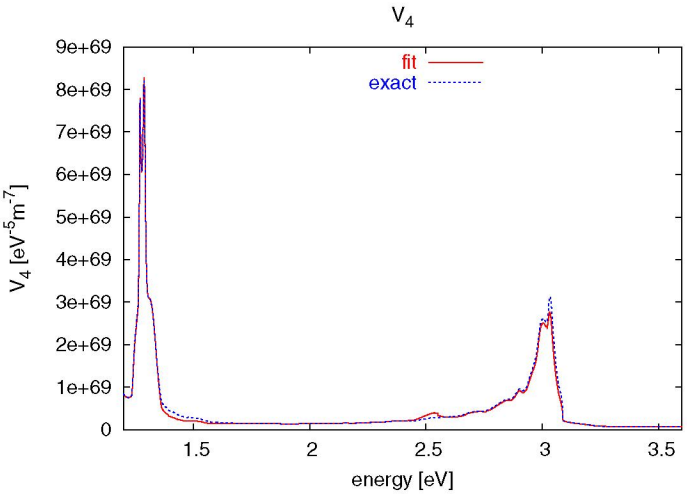

Fig. 5. V_4 contributing by HH and LH bands

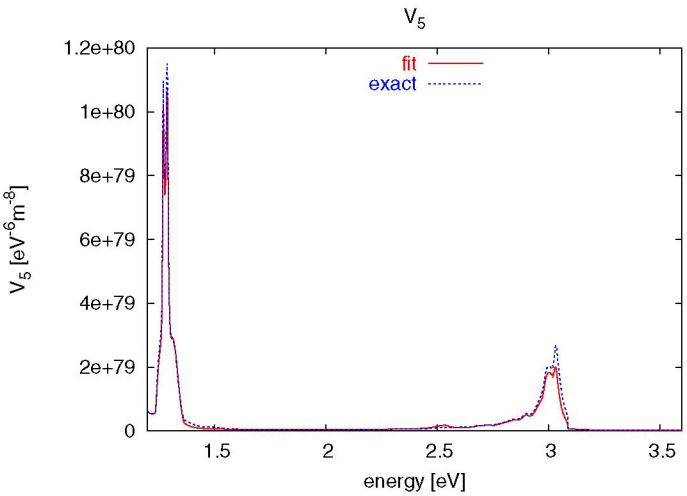

Fig. 6. V_5 contributing by HH and LH bands

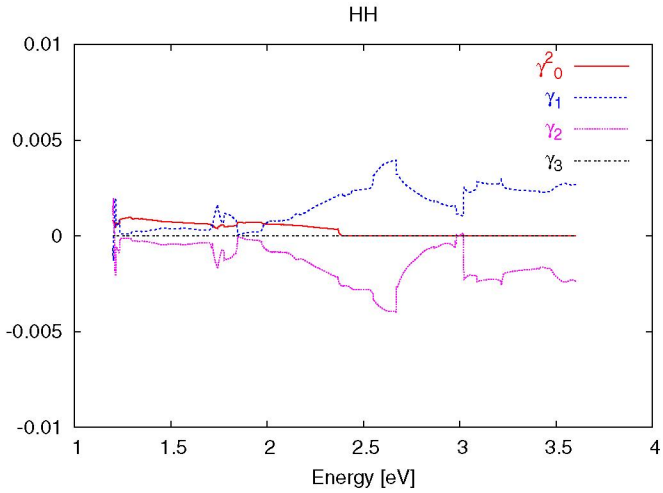

Fig. 7. Fitting parameters of HH band

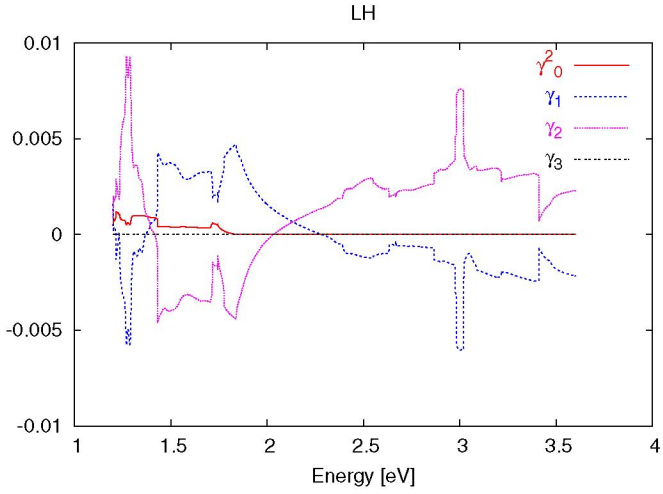

Fig. 8. Fitting parameters of LH band

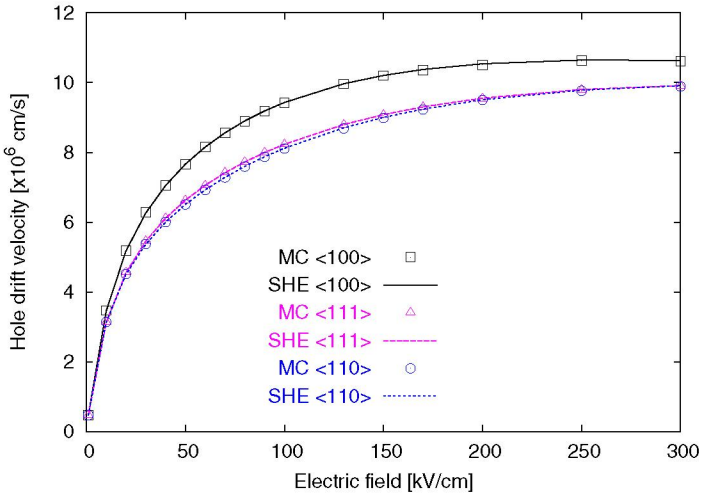

Fig. 9. Hole drift velocity v.s electric fields applied on different directions, without II

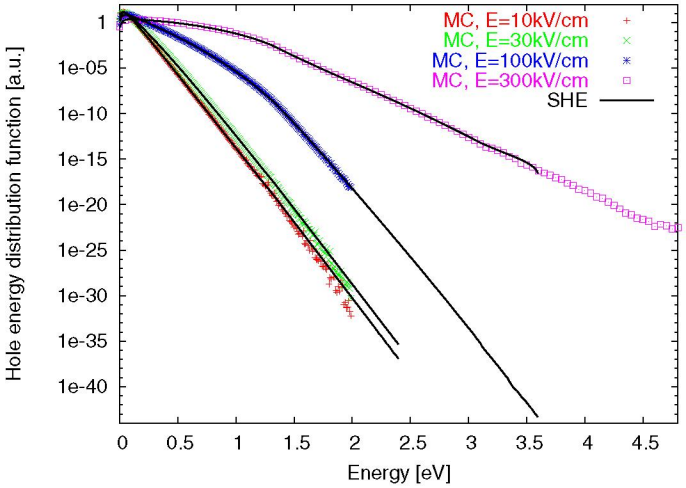

Fig. 10. Hole energy distribution function without II (applied electric fields in $\langle 110 \rangle$ direction)

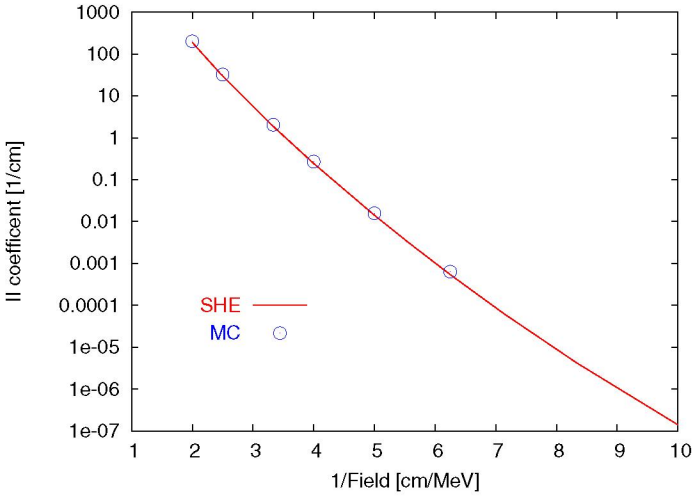

Fig. 11. Impact ionization coefficient (applied electric fields in $\langle 100 \rangle$ direction)

