

VISTA Status Report June 2000

K. Dragosits, C. Harlander, R. Kosik, H. Kosina, M. Nedjalkov, S. Selberherr



Institute for Microelectronics Technical University Vienna Gusshausstrasse 27-29 A-1040 Vienna, Austria

Contents

1	Sma	Small Signal Analysis of the Boltzmann Equation 1		
	1.1	Introduction	1	
	1.2	Basic Equations	1	
	1.3	The Monte Carlo Algorithm	2	
	1.4	Results and Discussion	2	
2	A Ba	ackward Monte Carlo Method	6	
	2.1	Introduction	6	
	2.2	Integral Forms	7	
	2.3	Results and Discussions	8	
	2.4	Physical Aspects	8	
	2.5	Numerical Aspects	8	
3	On t	the Interplay between Meshing and Discretization 12	2	
	3.1	Motivation	2	
	3.2	Diffusion	2	
	3.3	Physical Soundness	2	
		3.3.1 The Maximum Principle	2	
		3.3.2 Positive Transmissibility Condition	3	
	3.4	Finite Volumes versus Finite Elements	4	
	3.5	Natural Meshing Constraints	6	
	3.6	Distinctive Mesh Examples	8	
		3.6.1 Basic Mesh Construction	8	
		3.6.2 A Non-Delaunay Mesh Suitable for FE	9	
		3.6.3 Heuristics	1	
	3.7	Discussion	1	
		3.7.1 The Abstract Viewpoint	1	
		3.7.2 Practical Strategies	1	
		3.7.3 Nonlinear Case	2	
	3.8	Resume	2	

4	Two-Dimensional Simulation of Ferroelectric Materials24					
	4.1	Introdu	uction	24		
	4.2	Model	ing	24		
		4.2.1	Two-Dimensional Model	24		
		4.2.2	Hysteresis Model	24		
		4.2.3	Transient Model	26		
	4.3	Examp	ples	26		
		4.3.1	Extraction of Equivalent Parameters of a Finger Structure	27		
		4.3.2	Switching of a capacitor	29		
5	Indu	uctance	Calculation in Interconnect Structures	32		
	5.1	Introdu	uction	32		
	5.2	Physic	al approach	32		
	5.3	Impler	nentation	33		
		5.3.1	The Program Package SAP	33		
		5.3.2	Mutual Inductances	34		
		5.3.3	Self Inductances	34		

1 A Monte Carlo Method for Small Signal Analysis of the Boltzmann Equation

1.1 Introduction

Understanding the MC method as a versatile tool to solve integral equations enables its application to a class of problems which are not accessible by purely physically-based, imitative MC methods. In electrical engineering the linear small signal analysis of nonlinear systems plays an important role. Whether the linearized system is analyzed in the frequency or time domain is just a matter of convenience since the system responses obtained in either domain are linked by the Fourier transform.

At present, linear small signal analysis of semiconductor devices by the MC method is beyond the state of the art. However, recently progress has been made in performing MC small signal analysis of bulk carrier transport [1].

1.2 Basic Equations

Choosing a formulation in the time domain, a small perturbation \mathbf{E}_1 is superimposed to a stationary field \mathbf{E}_s . The stationary distribution function f_s will thus be perturbed by some small quantity f_1 .

$$\mathbf{E}(t) = \mathbf{E}_s + \mathbf{E}_1(t) \tag{1}$$

$$f(\mathbf{k},t) = f_s(\mathbf{k}) + f_1(\mathbf{k},t)$$
(2)

Inserting this Ansatz into the transient Boltzmann equation (BE) and retaining only first order perturbation terms yield a Boltzmann-like equation for f_1 which is linear in the perturbation \mathbf{E}_1 .

$$\frac{\partial f_1(\mathbf{k},t)}{\partial t} + \frac{q}{\hbar} \mathbf{E}_s \cdot \nabla f_1(\mathbf{k},t) = Q[f_1](\mathbf{k},t) - \frac{q}{\hbar} \mathbf{E}_1(t) \cdot \nabla f_s(\mathbf{k})$$
(3)

Compared with the common BE, (3) has an additional term on the right hand side which contains f_s , the solution of the stationary BE. The integro-differential type of equation, (3), is transformed into an integral form. Assuming an impulse-like excitation $\mathbf{E}_1(t) = \delta(t)\mathbf{E}_{im}$ results in the following integral equation for the impulse response f_1 .

$$f_1(\mathbf{k},t) = \int_0^t \mathrm{d}t' \int \mathrm{d}\mathbf{k}' f_1(\mathbf{k}',t') S(\mathbf{k}',\mathbf{K}(t')) \mathrm{e}^{-\int_{t'}^t \lambda(\mathbf{K}(y)dy)} + G(\mathbf{K}(0)) \mathrm{e}^{-\int_0^t \lambda(\mathbf{K}(y)dy)}$$
(4)

$$G(\mathbf{k}) = -\frac{q}{\hbar} \mathbf{E}_{\rm im} \cdot \nabla f_s(\mathbf{k}) \tag{5}$$

The free term of (4) is formally equivalent to the free term of the BE. The only difference is that G takes on also negative values, and can therefore not be interpreted as an initial distribution. In [2] G is expressed as a difference of two positive functions, $G = G^+ - G^-$, an Ansatz which decomposes (4) into two common BE for the unknowns f_1^+ and f_1^- . The initial conditions of these BE are $f_1^{\pm}(\mathbf{k}, 0) = G^{\pm}(\mathbf{k}) \ge 0$. In this way the impulse response is understood in terms of the concurrent evolution of two carrier ensembles.

Using different methods to generate the initial distributions of the two ensembles gives rise to a variety of MC algorithms. Both existing and new MC algorithms are obtained in a unified way, and a transparent, physical interpretation of the algorithms is supported.

1.3 The Monte Carlo Algorithm

In the case that the stationary and the small signal field vectors are collinear, the stationary BE can be used to express the distribution function gradient as

$$G(\mathbf{k}) = \frac{E_{\rm im}}{E_s} \left(\lambda(\mathbf{k}) f_s(\mathbf{k}) - \int f_s(\mathbf{k}') S(\mathbf{k}', \mathbf{k}) \mathrm{d}\mathbf{k}' \right) \,, \tag{6}$$

which gives a natural splitting of G into two positive functions. In the following we adopt the notation that terms which are employed in the respective algorithm as a probability density are enclosed in curly brackets.

From (6) we choose the initial distributions as

$$G^{+}(\mathbf{k}) = \frac{E_{\rm im}}{E_s} \langle \lambda \rangle_s \left\{ \frac{\lambda(\mathbf{k}) f_s(\mathbf{k})}{\langle \lambda \rangle_s} \right\}$$
(7)

$$G^{-}(\mathbf{k}') = \frac{E_{\rm im}}{E_s} \langle \lambda \rangle_s \int \left\{ \frac{\lambda(\mathbf{k}) f_s(\mathbf{k})}{\langle \lambda \rangle_s} \right\} \left\{ \frac{S(\mathbf{k}, \mathbf{k}')}{\lambda(\mathbf{k})} \right\} d\mathbf{k}$$
(8)

where $\langle \lambda \rangle_s = \int f_s(\mathbf{k})\lambda(\mathbf{k})d\mathbf{k}$ is introduced in the denominators to ensure normalization. $\langle \lambda \rangle_s$ is the inverse of the mean free-flight time, which can be seen immediately when evaluating the average by means of the 'before-scattering' method. The probability density $\lambda f_s / \langle \lambda \rangle_s$ represents the normalized distribution function of the before-scattering states. Consequently, the product of the two densities in (8) represents the normalized distribution function of the after-scattering states. Using the above expression the following algorithm can be formulated.

- 1) Follow a main trajectory for one free flight, store the before-scattering state in \mathbf{k}_b , and realize a scattering event from \mathbf{k}_b to \mathbf{k}_a .
- 2) Start a trajectory $\mathbf{K}^+(t)$ from \mathbf{k}_b and another trajectory $\mathbf{K}^-(t)$ from \mathbf{k}_a .
- 3) Follow both trajectories for time T. At equidistant times t_i add $A(\mathbf{K}^+(t_i))$ to a histogram ν_i^+ and $A(\mathbf{K}^-(t_i))$ to a histogram ν_i^- .
- 4) Continue with the first step until N k-points have been generated.
- 5) Calculate the time discrete impulse response as $\langle A \rangle_{im}(t_i) = \frac{E_{im} \langle \lambda \rangle_s}{NE_s} (\nu_i^+ \nu_i^-).$

The mean free-flight time must be additionally calculated during the simulation. This algorithm shows in a transparent way the evolution of the P and M ensembles, as well as the generation of the initial states for those ensembles.

1.4 Results and Discussion

The following simulation results are obtained by using the new Monte Carlo algorithm. Typical conditions for electrons in Si are considered as well as a special carrier dynamics feature, the Transit Time Resonance (TTR) effect [3][4] for electrons in GaAs. While Si is simulated at 300K, for GaAs the temperature is reduced to 10K to make the TTR effect clearly visible.

Analytical band models are adopted for both Si and GaAs, accounting for isotropic and non-parabolic conduction band valleys. For Si six equivalent X-valleys and for GaAs a three-valley model are included.



Figure 1: Impulse response of the differential energy.



The used phonon scattering rates can be found, for example, in [5]. Overlap integrals are neglected, and acoustic deformation potential scattering is assumed elastic.

Fig. 1 and Fig. 2 show the time response of the differential electron energy $\partial \langle \epsilon \rangle_{\rm im} / \partial E_{\rm im}$ and the longitudinal differential velocity $\partial \langle v \rangle_{\rm im} / \partial E_{\rm im}$ for Si at different field strengths. The response characteristics tend to zero when the two ensembles approach the steady state. The characteristic time associated with the relaxation process depicted Fig. 2, namely the momentum relaxation time, clearly decreases with increasing field. This effect is anticipated since the electron mobility $\mu = e\tau_m/m^*$ is known to show such a field reduction. Generally, within a few ps the steady state is reached by the two ensembles.



Figure 3: Real part of the differential velocity spectra.

Figure 4: Imaginary part of the differential velocity spectra.

Fig. 3 and Fig. 4 show the frequency dependence of the differential velocity obtained by a Fourier transform of the impulse response. The low frequency limits of the imaginary parts tend to zero, while the real parts tend to the corresponding differential mobility values $\partial \langle v \rangle_s / \partial E_s$.

For electrons in GaAs the assumed physical conditions are T = 10K and $E_s = 120V/cm$. In this case all electrons are in the Γ valley. In Fig. 5 the differential velocity and differential energy are presented normalized to the respective initial values. The impulse response characteristics reveal a damped oscillation. The pattern is pronounced also in the step response functions on Fig. 6 and Fig. 7, obtained by time integration of the corresponding impulse response functions.



Figure 5: Impulse response of the normalized differential energy and velocity.



Figure 6: Step response of the differential velocity.

The pattern appears to be independent of the concrete physical quantity, which leads to the conclusion that a peculiarity of the carrier dynamics is responsible for the behavior. The chosen physical conditions determine a peculiar behavior of the electrons already in the steady-state. Since the acoustical phonon scattering is low (below one scattering for 100ps), the electrons are accelerated by the field until they reach energies above the polar-optical phonon energy (0.036 eV). Above this energy the scattering rate for phonon emission increases rapidly, so that the electrons, penetrating the phonon threshold are intensively scattered back to energies close to zero.

The effect can most conveniently be discussed in the energy domain. The field impulse instantaneously creates a perturbation, represented by ensembles P and M with initial distributions G^+ and G^- , respectively. Fig. 8 shows the distributions as two peaks, located close to E = 0 and above the phonon threshold. The M ensemble is accelerated by the field towards the phonon threshold. The P ensemble is intensively transferred within less than two ps back to low energies and is then accelerated by the electric field.



Figure 7: Step response of the differential energy.

Figure 8: Energy distribution of the P and M ensembles at t = 0 and t = 8 ps.

Fig. 9 and Fig 10 show the individual evolution of the two ensembles. The initial peaks broaden towards the steady state which is reached at about 80 ps.

The *M* ensemble undergoes an evolution similar to that of the *P* ensemble, however with same delay. This is demonstrated in Fig. 8 where the two distribution functions are shown at t = 8ps. The time delay

1.4 Results and Discussion

in the evolution is responsible for the oscillation in $\langle A \rangle_{im}(t)$. If the two distributions were equivalent at a certain time, they would oscillate synchronously for later times and no oscillation in $\langle A \rangle_{im}(t)$ would show up.

For the considered condition each electron undergoes a permanent cycle in the energy domain. The TTR effect occurs since the two ensembles collectively follow this single particle behavior during a certain transition time.



Figure 9: Evolution of the distribution function of the P ensemble.



Figure 10: Evolution of the distribution function of the M ensemble.

2 A Backward Monte Carlo Method for Simulation of the Electron Quantum Kinetics in Semiconductors

2.1 Introduction

We introduce an equation which describes the quantum kinetics of a semiconductor carrier system coupled with a phonon bath. The time evolution of such system is predestinated by the initial state. On a quantum-kinetic level the knowledge of the carrier-phonon initial state is often a problematic task. In this respect it is convenient to consider carries generated by a laser pulse at low temperatures, a case with no carriers at the beginning of the excitation. The relevant description of the phenomena is given by the semiconductor Bloch equations accounting for the carrier-phonon, carrier-photon and carriercarrier interactions and interference effects [6]. In order to concentrate on the carrier-phonon kinetics only, a simplified consideration is needed, given by the one-band model [7]. It describes a relaxation of an initial distribution of carriers i.e. the phonon interaction is switched on after the laser pulse completed the carrier generation. Despite that a generation term is more realistic than the initial condition, the latter allows to concentrate on the quantum-kinetic aspects of the electron-phonon interaction. The one-band model is obtained in the framework of the density matrix formalism. The Hamiltonian $H = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} + \sum_{\mathbf{q}} \omega b_{\mathbf{q}}^{\dagger} b_{\mathbf{q}} + \sum_{\mathbf{k}', \mathbf{k}} \left(g_{\mathbf{q}} c_{\mathbf{k}'}^{\dagger} b_{\mathbf{k}'-\mathbf{k}} c_{\mathbf{k}} + cc \right)$ accounts for Froehlich interaction with coupling $g_{\mathbf{k}'-\mathbf{k}}$, $c_{\mathbf{k}}^{\dagger}$ ($c_{\mathbf{k}}$) and $b_{\mathbf{q}}^{\dagger}$ ($b_{\mathbf{q}}$) are the electron and phonon creation (annihilation) operators respectively. tively, $\epsilon_{\mathbf{k}} = \hbar^2 k^2 / 2m$ is the electron energy, and ω is the phonon frequency. The physical variables are statistical averages $\langle \cdot \rangle$ of combinations of creation and annihilation operators. Relevant are the electron and phonon distributions $f(\mathbf{k},t) = \langle c_{\mathbf{k}}^+ c_{\mathbf{k}} \rangle$, $n_q(\mathbf{q},t) = \langle b_{\mathbf{q}}^+ b_{\mathbf{q}} \rangle$, Their equations of motion introduce the phonon assisted density matrices $s(\mathbf{k}', \mathbf{k}, t) = \frac{i}{\hbar}g_{\mathbf{k}'-\mathbf{k}}\langle c_{\mathbf{k}'}^+ b_{\mathbf{k}'-\mathbf{k}}c_{\mathbf{k}}\rangle$. The equations for s introduce averages of four operators and so forth, leading to an infinite set (the BBGKY hierarchy) of equations. The set is closed by approximations in the equations of motion of the four operator averages. First the five operator terms are factorized into distribution functions and phonon assisted density matrices. Afterwards adiabatic and Markov approximations are performed and the result is used in the equations for s. The linearized one-band model, under the assumption of equilibrium phonons is given by the equations:

$$\frac{d}{dt}f(\mathbf{k},t) = 2\sum_{\mathbf{k}'} Re[s(\mathbf{k}',\mathbf{k},t) - s(\mathbf{k},\mathbf{k}',t)]$$

$$\frac{d}{dt}s(\mathbf{k}',\mathbf{k},t) = (i\Omega(\mathbf{k}',\mathbf{k}) - \Gamma(\mathbf{k}',\mathbf{k}))s(\mathbf{k}',\mathbf{k},t) + \frac{1}{\hbar^2} ||g_{\mathbf{k}'-\mathbf{k}}||^2 [f(\mathbf{k}',t)(n+1) - f(\mathbf{k},t)n] (10)$$

which are supplemented by initial conditions $f(\mathbf{k}, 0) = \phi(\mathbf{k}), s(\mathbf{k}', \mathbf{k}, 0) = 0$.

Here $\Omega(\mathbf{k}', \mathbf{k}) = (\epsilon(\mathbf{k}') - \epsilon(\mathbf{k}) - \hbar\omega)/\hbar$, *n* is the Bose distribution, the damping $\Gamma(\mathbf{k}', \mathbf{k}) = \lambda(\mathbf{k}) + \lambda(\mathbf{k}')$ is related to the finite carrier lifetime against the scattering process: $\lambda(\mathbf{k}) = \int d^3q \frac{V}{2^3\pi^2\hbar} \sum_{\pm} ||g_{\mathbf{k}'-\mathbf{k}}||^2 \delta(\epsilon(\mathbf{k}') - \epsilon(\mathbf{k}) \pm \hbar\omega)(n + 1/2 \pm 1/2)$. This equation set can be further processed [8] if (10) is integrated formally and inserted in (9) which leads to:

$$\frac{\partial}{\partial t'} f(\mathbf{k}, t') = \int_{0}^{t'} dt'' \int d\mathbf{k}' \{ S(\mathbf{k}', \mathbf{k}, t' - t'') f(\mathbf{k}', t'') - S(\mathbf{k}, \mathbf{k}', t' - t'') f(k, t'') \} \quad (11)$$

$$S(\mathbf{k}', \mathbf{k}, t' - t'') = \frac{V}{(2\pi)^{3} \hbar^{2}} \|g_{\mathbf{k}'-\mathbf{k}}\|^{2} e^{-(\Gamma(\mathbf{k}', \mathbf{k}))(t' - t'')} \times \{ \cos(\Omega(\mathbf{k}', \mathbf{k})(t' - t''))(n+1) + \cos(\Omega(\mathbf{k}, \mathbf{k}')(t' - t''))n \}$$

The result can be recognized as the zero electric field form of the quantum-kinetic equation reported in [9], which is now obtained by an alternative to the projection technique way.

It has been recognized that the numerical evaluation of (11) is a formidable task and that a relevant approach is the Monte Carlo (MC) method [9]. The numerical method used here is a formal extension of the Backward MC approach for semiclassical [10] and quantum transport [11] simulations. The method utilizes the theory of stochastic algorithms for solving integral equations. The convergence of iteration series of the concrete integral equation significantly affects the efficiency of the method. In the next section we introduce three different integral forms of (11). They allow to analyze a variety of physical and numerical aspects of the quantum-kinetic equation and the numerical method, presented in the last section.

2.2 Integral Forms

The first integral form of (11) is obtained by a direct integration over t' in the limits (0; t) and using the initial condition on the right hand side. The equation gives rise to a second integral form obtained after the following transformations. The order of the two time integrals can be exchanged according to $\int_0^t dt' \int_0^{t'} dt'' = \int_0^t dt'' \int_{t''}^t dt'$. Furthermore the kernel S can be analytically integrated over t' with the help of the identity:

$$\int_{0}^{t-t^{\prime}} d\tau e^{-(\Gamma(\mathbf{k}',\mathbf{k}))\tau} \cos(\Omega(\mathbf{k}',\mathbf{k})\tau) =$$

$$L(\mathbf{k}',\mathbf{k}) + L(\mathbf{k}',\mathbf{k}) \left(\frac{\Omega(\mathbf{k}',\mathbf{k})}{\Gamma(\mathbf{k}',\mathbf{k})} sin(\Omega(\mathbf{k}',\mathbf{k})(t-t'')) - \cos(\Omega(\mathbf{k}',\mathbf{k})(t-t''))\right) e^{-(\Gamma(\mathbf{k}',\mathbf{k}))(t-t'')}$$
(12)

where L is a Lorentzian function $L(\mathbf{k}', \mathbf{k}) = \frac{\Gamma(\mathbf{k}', \mathbf{k})}{\Omega^2(\mathbf{k}', \mathbf{k}) + \Gamma^2(\mathbf{k}', \mathbf{k})}$. Thus the scattering term denoted by $\mathcal{L}(\Gamma(\mathbf{k}', \mathbf{k}); \mathbf{k}', \mathbf{k}, t - t'') = \int_{t''}^{t} dt' S(\mathbf{k}', \mathbf{k}, t' - t'')$ is decomposed into a time independent part (two Lorentzian multiplied by the equilibrium phonon factors) and an oscillating, exponentially damped function of the evolution time. The two parts cancel each other at t = 0. The Markovian limit $t \to \infty$ of \mathcal{L} is presented by the Lorentzian part. The time dependent part is liable for the memory character of the equation.

$$f(\mathbf{k},t) = \int_0^t dt'' \int d\mathbf{k}' \left(\mathcal{L}(\Gamma(\mathbf{k}',\mathbf{k});\mathbf{k}',\mathbf{k},t-t'') f(\mathbf{k}',t'') - \mathcal{L}(\Gamma(\mathbf{k}',\mathbf{k});\mathbf{k},\mathbf{k}',t-t'') f(\mathbf{k},t'') \right) + \phi(k)$$
(13)

The Markovian limit of this equation does not recover the semiclassical Boltzmann equation. It is due to the finite lifetime of the carriers - the energy conserving delta function is recovered by the limit $\Gamma \rightarrow 0$.

The derivation of the third integral form utilizes the main idea of the path integral transformation, which is the basis of the MC calculations in the Boltzmann transport framework. A term $\psi(\mathbf{k}) f(\mathbf{k}, t')$, where ψ is a positive function is added to both sides of (11). The left hand side can be written as $e^{-\psi(\mathbf{k})t'} \frac{d}{dt'} \left(e^{\psi(\mathbf{k})t'} f(\mathbf{k}, t') \right)$. The equation is further divided by $e^{-\psi(\mathbf{k})t'}$ and integrated on t' in the interval (0; t). A subsequent division on $e^{\psi(\mathbf{k})t}$ leads to a path integral formulation, with $f(\mathbf{k}, t)$ on the left and the exponential damping due to the ψ function incorporated in the time integrals on the right. The identity (12) still can be applied to give:

$$f(\mathbf{k},t) = \int_0^t dt'' \int d\mathbf{k}' e^{-\psi(\mathbf{k})(t-t'')} \mathcal{L}(\Gamma(\mathbf{k}',\mathbf{k}) - \psi(\mathbf{k});\mathbf{k}',\mathbf{k},t-t'') f(\mathbf{k}',t'') -$$
(14)

$$\int_0^t dt'' e^{-\psi(\mathbf{k})(t-t'')} \left(\int d\mathbf{k}' \mathcal{L}(\Gamma(\mathbf{k}',\mathbf{k}) - \psi(\mathbf{k});\mathbf{k},\mathbf{k}',t-t'') - \psi(\mathbf{k}) \right) f(\mathbf{k},t'') + \phi(k) e^{-\psi(\mathbf{k})}$$

This path integral form coincides with the zero field Barker-Ferry equation [9] with the only modification, that the self-scattering constant is replaced by the function ψ . The advantages of the Barker-Ferry form for the utilized numerical approach are analyzed in the next section. The physical aspects of the quantum model and particularly of its Lorentzian limit are discussed and demonstrated by simulation experiments.

2.3 Results and Discussions

The simulation results are obtained for GaAs with material parameters taken from [7]. The initial condition is given by a Gaussian distribution in energy, corresponding to a 87 femtosecond laser pulse with an excess energy of 180 meV, scaled in a way to ensure peak value equal to unity. Zero lattice temperature has been chosen in order to allow a convenient comparison with the behavior of semiclassical electrons. At such temperature the latter can only emit phonons and loose energy equal to a multiple of the phonon energy $\hbar\omega$. The evolution of the distribution function is patterned by replicas of the initial distribution shifted towards low energies. The electrons can not be scattered out of the states below the phonon energy and can not appear above the initial distribution. This simple semiclassical behavior will be the reference background for the effects imposed by the quantum-kinetic equation (11). The symmetry of the task allows to use spherical coordinates with a wave vector amplitude $k = |\mathbf{k}|$. The figures present the quantity kf(k,t), the distribution function multiplied by the density of states, in arbitrary units versus k^2 $(10^{14}/m^2)$, which is proportional to the electron energy.

2.4 Physical Aspects

Figure 1 shows quantum solutions for low evolution times. Electrons appear in the semiclasically forbidden region above the initial condition. This is explained by referring to the scattering term S in the first integral form. For small time differences in the cosine function the probability for scattering into the whole Brillouin zone becomes finite. Despite that only a small fraction of the electrons populate the higher energy states - the resolution is within four orders of magnitude below the initial peak value - this property remains even if a generation term is considered. The initial condition allows a clear demonstration of the effect.

The quantum effects in the energy region below the initial condition can be interpreted with the help of the scattering term \mathcal{L} of the second integral form. Itself the time independent part of \mathcal{L} is responsible for the effect of collisional broadening, destroying the replica-like pattern of the distribution function. Figure 2 compares the semiclassical distribution after 400fs with the solution of a Boltzmann like equation (BLE), where the delta function in energy is replaced by the Lorentzian. A detailed discussion of the effects delivered by the Lorentzian model are given in [12].

The memory character of the equation, carried on by the time-dependent part of \mathcal{L} , introduces a collision retardation. The latter is demonstrated in Figures 3 and 4 as an delay in the build up of the remote peaks of the quantum solutions as compared to the corresponding BLE solutions.

At high evolution times the time independent part dominates the kinetics and introduces additional deviations from the semiclassical behavior. Due to the long reaching tails of the Lorentzian function, the electrons with energy below the LO phonon threshold are in mutual exchange, having an out-scattering rate of order of $10^{-5}/fs$. Furthermore a fraction of electrons run away towards the high energy states leading to an artificial heating of the electron system [12]. Thus the application of (11) for high evolution times must be handled with care.

2.5 Numerical Aspects

The applied Monte Carlo method is based on the following estimator:

$$\nu_i(x_0) = \frac{\mathcal{K}(x_0, x_1)}{P(x_0, x_1)} \dots \frac{\mathcal{K}(x_{i-1}, x_i)}{P(x_{i-1}, x_i)} \phi(x_i)$$

which calculates the multiple integrals forming the iteration series of the integral equation: $f(x) = \int dx' \mathcal{K}(x,x') f(x') + \phi(x)$,[8]. Here x_0 is the desired point k, t where the solution is to be evaluated and x_i , i > 0 given by the set of the integral variables: k', t', t'' for the first form and k', t'' for the second and third form and the BLE. An even transition probability density P has been chosen for the all variables in the first form. For the rest of the equations k has a Lorentzian distribution in the phase space, and the time is generated according the exponential distribution. The advantages of the method lie in the direct evaluation of the functional value at the desired point - in contrast the Ensemble MC provides only averaged estimates. A direct control of the numerical precision in the desired point is available. This is demonstrated by the high resolution of the statistical results on Figure 1. The method does not require the knowledge of the distribution function dependence on k at previous times.

The variance of the estimator for the first integral form rapidly increases, allowing simulations up to 100fs evolution time. The mean value of the estimator is formed by cancellations of positive and negative numbers, which rapidly increase with the evolution time. The analytic evaluation of one time integral leading to the second integral form only slightly improves the variance. This shows that the reason is in the poor convergence of the iteration series rather than in the stochastic error in the evaluation of the integrals. The build up of the Markovian limit of (12) increases the number of the relevant iteration terms before the truncation of the series. The same problem has been reported for the direct time integral form of the Boltzmann equation [11]. The remedy in the semiclassical case is in the path integral formulation of the equation, giving the probability for the free-flight time. The same effect is observed in the path integral form (14). The function ψ subtracted from the second term gives rise to an exponential damping with the evolution time, which improves the convergence of the iteration series. The above analysis is supported by the numerical experiments. A choice of $\psi = \lambda$ has been done, which simplifies the scattering term. Despite that the Lorentzian in (14) have higher peak values as compared to (12), evolution times of 300fs can be conveniently simulated. For the BLE ψ has been chosen to cancel exactly the out-scattering term.



Figure 11: Quantum solutions for three low evolution times. Electrons appear in the semiclasically forbidden region above the initial condition.



Figure 12: Semiclassical and BLE solutions for 400fs evolution time. The Lorentzian destroys the peak-like pattern in the region of low energies.



Figure 13: Quantum and BLE solutions for 150fs evolution time. The quantum solution follows the BLE solution with a delay.



Figure 14: Quantum and BLE solutions for 200fs and 300fs evolution time.

3 On the Interplay between Meshing and Discretization in Three-Dimensional Diffusion Simulation

3.1 Motivation

Continuum based diffusion and dopant activation models are among the dominant tools used to investigate and understand integrated circuit process development.

A major part of model development and simulation are still done in one and two dimensions. This is due to metrological reasons and the enormous numerical costs for a complex three-dimensional model. Besides this, an additional factor makes simulation in three dimensions very difficult, namely strong constraints on meshing. The purpose of our article is a fundamental one: To clarify the nature of the proper constraints on the mesh which will ensure a good quality of the solution.

3.2 Diffusion

The well known model equation for diffusion is

$$\frac{\partial C}{\partial t} = \nabla \cdot D\nabla C,\tag{15}$$

where C denotes the concentration and D is called diffusion coefficient or diffusivity.

In general, the diffusion models used in semiconductor process simulation are strongly nonlinear because the diffusion coefficients depend, e.g., on the impurity and point defect concentrations. These dependences also couple the equations for multiple impurities and point defects. Additionally, more complex models include chemical reactions and contain convection terms.

The actual physical diffusion mechanisms in semiconductor manufacturing processes are a topic of active research (see [13] for a special example or [14], Chapter on "Modeling and Simulation", for wishful thinking). As a basis there is the entropy principle, universally valid for any assumed physical model: The flow must always go from regions of high concentrations to regions where the concentration is low. Evolving in time, the concentration must smooth out to an equilibrium distribution. It is desirable that the simulation mirrors this physical behavior. However, this is far from being a trivial task.

3.3 Physical Soundness

3.3.1 The Maximum Principle

In the case of diffusion physical soundness of the solution finds its concise expression in the maximum principle for parabolic differential operators.

Let D denote a finite open domain in \mathbb{R}^m with smooth boundary ∂D , \overline{D} its closure. For each T > 0, let $D_T = (0,T] \times D$, $S_T = (0,T] \times \partial D$. Let $C^0(\overline{D_T})$ denote the set of all functions continuous on $\overline{D_T}$, $C^{1,2}(D_T)$ the set of all functions which are once continuously differentiable in t and twice continuously differentiable in x for all $(t, x) \in D_T$.

Then the maximum principle for parabolic differential operators can be stated as follows [15] [16]: Let u be a non-constant function,

$$u \in C^{1,2}(D_T) \cap C^0(\overline{D_T}), \tag{16}$$

3.3 Physical Soundness

which satisfies

$$\frac{\partial u}{\partial t} - Lu \le 0 \quad \text{in} \quad D_T, \tag{17}$$

where L is a uniformly elliptic operator with bounded coefficients (e.g., the Laplace operator). Then u can attain its maximum only for t = 0 or on the boundary ∂D of D. Furthermore, if u attains its maximum m at some point (t_m, x_m) of S_T then

$$\frac{\partial u}{\partial \nu}(t_m, x_m) > 0, \tag{18}$$

where $\frac{\partial}{\partial \nu}$ denotes the outward normal derivative.

Physically, this means that the maximum occurs at the initial time or at the boundary. In the latter case some flow from outside must exist at the point of maximum.

The dual minimum principle states that the minimum occurs at the initial time or at the boundary. In the latter case some flow to the outside must exist.

If homogeneous Neumann boundary conditions

$$\frac{\partial u}{\partial \nu} = 0 \qquad (\text{on } S_T) \tag{19}$$

and a continuous initial distribution $u_0(0, x)$ are prescribed to the partial differential equation

$$\frac{\partial u}{\partial t} - Lu = 0 \qquad (\text{on } D_T) \tag{20}$$

the combined minmax principle guarantees that the concentration will stay below the initial maximum value and above the initial minimum value for all times, as extrema can only occur for t = 0.

3.3.2 Positive Transmissibility Condition

The parameters of the discretization of a partial differential equation (PDE) have to be chosen in a way that the most characteristic physical properties are maintained.

Assuming a suitable mass conserving node based discretization (e.g., finite differences, finite elements with lumping mass, finite boxes), the discretized diffusion equation can be written as a system of equations of the form

$$w_i \frac{\Delta C^i}{\Delta t} + \sum_j \gamma_{ij} C_n^j = 0, \qquad (21)$$

where $w_i > 0$ and γ_{ij} denote real coefficients, C_n^i is the concentration value on node *i* after timestep *n* and (using backwards Euler)

$$\frac{\Delta C^{i}}{\Delta t} = \frac{C_{n}^{i} - C_{n-1}^{i}}{t_{n} - t_{n-1}}.$$
(22)

Then it follows that the discrete solution will satisfy a minmax principle if the matrix γ resulting from the discretization is an M-matrix [17], i.e., a real, nonsingular $n \times n$ matrix A where

$$a_{ij} \le 0 \quad \forall i \ne j \tag{23}$$

and

$$4^{-1} \ge 0, \tag{24}$$

which means that all elements of A^{-1} are greater or equal to zero.

Constraint (23) has a physical interpretation in terms of a positive transmissibility condition [18]: Rewriting Equation (21) gives

$$w_i \frac{\Delta C^i}{\Delta t} = \sum_{j \neq i} \gamma_{ij} (C_n^i - C_n^j) - (\sum_j \gamma_{ij}) C_n^i.$$
⁽²⁵⁾

Here $\gamma_{ij}(C_n^i - C_n^j)$ can be interpreted as the amount of mass transferred from node j to node i per time unit. The physical flow has to be directed from higher to lower concentrations, which requires

$$\gamma_{ij} \le 0 \quad \forall i \neq j \tag{26}$$

and this corresponds to Condition (23).

The violation of the maximum principle in simulation results can be detected by the emergence of negative concentrations and spurious oscillations which are caused by negative transmissibilities and the resulting non-physical flows.

3.4 Finite Volumes versus Finite Elements

The popular discretization schemes for PDEs in complicated domains can be divided into two species: finite element and finite volume (finite box) methods.

We compare finite volumes (FV) and finite elements (FE) with respect to the constraints they impose on the mesh to achieve positive transmissibilities and hence a discrete minmax principle.

For the theoretical analysis of the possible discretization schemes, we concentrate on the model case (15) with constant diffusivity D.

For both FV and FE we use the standard approaches with backwards Euler time discretization [19]. In the case of FE we use the Galerkin approach with linear shape functions and lumping mass.

In two dimensions finite elements and finite boxes give exactly the same discretization, if in the case of finite elements the mass matrix is lumped [20]. Therefore the usage of a customary Delaunay mesh guarantees that the solution does not contain any non-physical negative concentrations [21].

In three dimensions the situation changes drastically, since the good properties of FE on a Delaunay mesh are lost. We will analyze and explain the meaning of this in practical and theoretical terms. In this section we will make the beginning and show simulation results demonstrating what "loss of good properties" means in purely practical terms. Section 3.5 contains a theoretical analysis and gives the abstract theory behind the problem. Finally, Section 3.6 analyzes in detail the examples of this section using the machinery developed in Section 3.5.

The simulations were done using AMIGOS [22], a general purpose PDE solver and integrated model development environment. All simulations are done on one and the same three-dimensional Delaunay mesh. The rather coarse mesh is derived from an ortho-product point distribution ($21 \times 21 \times 21$ points) on a cubic simulation domain, whereby every sub-cube is tetrahedralized into six tetrahedra. The mesh is depicted in Fig. 23 (see also Fig. 21), its theoretical properties are analyzed in Section 3.6.

The initial distribution exhibits radial symmetry (Fig. 15) given by a two-dimensional Gaussian profile (offset 10^{12}). Homogeneous Neumann boundary conditions are prescribed on the whole boundary.

The example is chosen to illustrate the fundamental qualitative difference between two and three dimensions for finite element diffusion simulations. A good discretization should approximately conserve the independence of z and the symmetry of the initial distribution when it evolves in time. Note that even in the continuous case the rotational symmetry is broken by the cubic boundary.



The visualization of the three-dimensional concentration distribution is accommodated to the symmetry by use of a planar cut in the xy-plane combined with a cylindrical cut in z-direction.

Fig. 16 shows the FE solution after 3000s. The concentration has fallen below the initial minimum value on large areas. The emergence of negative concentrations is demonstrated by the black patterns on the figure. All symmetries are lost, most remarkably the independence of z is not preserved. The latter is shown on Fig. 17 where the viewpoint is rotated 90 degrees. The negative areas spread out in time as seen when comparing Fig. 17 and Fig. 18.

The solution produced by FE is qualitatively not satisfactory and even incorrect on a macroscopic scale. This is opposed by the FV solution (Fig. 19) which preserves the symmetry and fulfills the critical minmax principle. Marginal violation of the independence of the solution of z is due to rounding and interpolation errors.

Finally, Fig. 20 displays the absolute error (FV solution minus FE solution) between FE and FV and depicts a global anisotropy.

In a two-dimensional FE simulation of the same problem none of the effects described above can be observed when a Delaunay mesh is used. The examples in this section were based on an ortho-grid for ease of theoretical analysis in Section 3.6. As a side effect they also show that naive use (choice of a "bad" Delaunay triangulation) of a mesh based on a structured grid can lead to large discretization errors.



Figure 17: FE after 3000 seconds. Independence of z is lost.



Figure 18: FE after 10000 seconds. The finite element disaster. Negative Concentrations have spread out.



Figure 19: FV after 10000 seconds. Preservation of the symmetry.

Figure 20: Absolute error between FE and FV. Global anisotropy.

3.5 **Natural Meshing Constraints**

The experiments above demonstrate a puzzling dependence of the quality of FE solutions on the dimension of the Delaunay mesh. While in two dimensions FE solutions exhibit good qualitative properties, in three dimensions the produced solutions can be a disaster. The aim of this section is to investigate the observed effects in terms of mesh requirements.

Already in two dimensions careless discretization (e.g., finite elements without lumping mass) and/or bad meshing (e.g., use of a non-Delaunay mesh) will result in non-physical flows and the emergence of negative concentrations, see [18] and [23].

In three dimensions the interplay between meshing and discretization is still more complicated. In many cases the discretizations rely on heavy constraints on the meshing strategy applied in order to achieve the desired properties.

In the simulations above we used the standard Galerkin approach for FE with linear shape functions and backwards Euler time discretization.

In this case the system matrix **K** is of the form

$$\mathbf{K} = \frac{1}{\Delta t} \mathbf{M} + D\mathbf{S} \tag{27}$$

where \mathbf{M} denotes the mass matrix, \mathbf{S} is the stiffness matrix, and D is the diffusion constant.

The discrete solution fulfills a maximum principle if the mass matrix is lumped and S is an M-matrix. The coefficients s_{ij} of S are given by

$$s_{ij} = \sum_{elements} \int_{e} \nabla N_i \cdot \nabla N_j \, dA \tag{28}$$

where N_i , N_j denote the shape functions and A is the area (volume) of element e. The sum runs over all elements e containing the edge e_{ij} . To make **S** an M-matrix the off-diagonal entries must not be positive:

$$s_{ij} \le 0, \quad i \ne j. \tag{29}$$

If the mesh has no obtuse angles, every term in the sum is negative and Condition (23) is trivially fulfilled. However, this is too strict.

The scalar product $(\nabla N_i \cdot \nabla N_j)$ has a simple geometrical meaning and allows a reinterpretation of the constraint (29) in basic geometrical terms using only the dihedral angles and the length of the edges.

Xu and Zikatanov [24] derive the following equivalent criterion which we name the (weighted) dihedral angle criterion:

Let e_{ij} be the edge connecting two vertices v_i and v_j in a three-dimensional mesh. In every tetrahedra t_k containing e_{ij} there exists a face opposite to v_i and a face opposite to v_j . The two faces span a dihedral angle θ_k and their intersection has length l_k . S is an M-matrix if and only if, for any fixed edge e_{ij} the following inequality is satisfied:

$$\sum_{k=1}^{n} l_k \cot \theta_k \ge 0, \tag{30}$$

where n is the number of tetrahedra adjacent to e_{ij} .

Fig. 21 displays the dihedral angles linked to the cube diagonal in a tessellation consisting of 6 tetrahedra.

The two-dimensional variant of (30) is

$$\cot \theta_1 + \cot \theta_2 \ge 0 \tag{31}$$

where θ_1 and θ_2 are the angles opposite to an edge e_{ij} which is shared by two triangles. This is equivalent to the Delaunay criterion [21] and explains the good properties of FE in two dimensions on Delaunay meshes.

3.6 Distinctive Mesh Examples

In three dimensions the dihedral angle and the Delaunay criterion are of quite diverse nature. Both constraints form the interesting case of two natural quality criteria, which are equivalent in two dimensions but split into different notions in three dimensions.

Our analysis is based on three specific mesh examples:

- **Mesh Example 1:** A Delaunay mesh which is not suitable as a finite element mesh for diffusion applications. This kind of mesh was used in the simulations above.
- Mesh Example 2: A Delaunay mesh which is suitable for finite element diffusion simulation.
- Mesh Example 3: A non-Delaunay mesh with obtuse dihedral angles which is still suitable as a finite element mesh.

The combination of these examples proves that in three dimensions the Delaunay criterion is neither sufficient nor necessary to achieve a maximum principle in finite element diffusion simulations.

3.6.1 Basic Mesh Construction

The examples were constructed by exploiting an ortho-product point distribution. A cube defined by eight points can be tetrahedralized in several different ways:

- T_6 Tessellation: A cube is composed of six tetrahedra (Fig. 21).
- T_5 Tessellation: A cube is composed of five tetrahedra (Fig. 22).

For the purpose of demonstration a specific tessellation T_6 (Fig. 21) is used which contains sliver elements with obtuse dihedral angles. (Note that also T_6 tessellations exist which do not contain obtuse angles.) The tessellation T_5 (Fig. 22) on the other hand does not contain such elements.

Meshes suitable for simulation are then built by stacking a large number of identically tessellated cubes (see Fig. 23 and Fig. 24). The typical characteristics of each tessellation type are thereby conserved.

All elements of both tessellations fulfill the empty circumsphere Delaunay criterion, because all points lie on the perimeter of the cube's circumsphere.

Because of the total absence of obtuse dihedral angles, the T_5 tessellation fulfills the dihedral angle criterion.

To test if this result is valid for the T_6 tessellation, we use AMIGOS to display the stiffness matrix and directly check the sign of the matrix entries. The stiffness matrix corresponding to a T_6 -tessellated cube is shown in Fig. 25 where the entries for the edge (3, 4) of the mesh are underlined. The global coupling coefficient has positive sign, which proves that the dihedral angle criterion is violated in this case.

Hence, both meshes are global Delaunay meshes and yet only one satisfies the dihedral angle criterion.

18



Figure 21: T_6 tessellation and the dihedral angle criterion (30).



Figure 23: Delaunay mesh built from T_6 tessellated cubes, dihedral angle criterion is not fulfilled.

3.6.2 A Non-Delaunay Mesh Suitable for FE

We try to construct a mesh, which is not Delaunay, but still fulfills the dihedral angle criterion. The key idea to its construction is to take the "good" T_5 mesh (which fulfills both the angle and the Delaunay criterion) and to modify it in such a way, that Delaunay is violated but the angle criterion is preserved [25].

As the T_5 mesh is a degenerate case with 8 cospherical points, violation of Delaunay is easily achieved by shifting points slightly (e.g., infinitesimally) in certain locations. This results in a non-Delaunay mesh which (by a simple continuity argument) still satisfies (30).

Fig. 26 shows a submesh consisting of eight cubes, which form the building blocks of the mesh in Fig. 27. The point in the middle (numbered "6"), which belongs to all eight cubes has been shifted downwards. The Delaunay criterion is violated, because the circumspheres of several unmodified tetrahedra contain the shifted point in its interior. The dashed lines in the figure mark two of the non-Delaunay triangles.



Figure 22: T_5 tessellation, no obtuse dihedral angles.



Figure 24: Delaunay mesh built from T_5 tessellated cubes, dihedral angle criterion is satisfied.



Figure 25: Global stiffness matrix for a T_6 tessellation and local matrices of those four elements which are adjacent to edge (3, 4).



Figure 26: T_5 type tessellation with a shifted point. Building block for mesh in Fig. 27.



Figure 27: Non-Delaunay mesh fulfilling the dihedral angle criterion.

The calculation for the entire mesh (Fig. 27) verifies, that the FE requirements for the stiffness matrix are fulfilled. The shifting of a point introduces obtuse dihedral angles and positive contributions to offdiagonal elements of the stiffness matrix. However, criterion (28) is satisfied and the global stiffness matrix remains an M-matrix.

3.7 Discussion

3.6.3 Heuristics

Our examples show that Delaunay neither implies nor is it implied by the dihedral angle criterion.

The former result was discussed in [21] where a Delaunay mesh unsuitable for FE simulation was presented. The construction of a simple mesh which fulfills the dihedral angle criterion but not the Delaunay criterion complements this previous research.

Heuristically the latter result was motivated by Putti's discovery (see Section 3.7.1) that finite elements give the same discretization as gravity boxes in three dimensions. Gravity boxes and Voronoi boxes are distinct notions. There is no sense in which a gravity box is a Voronoi box or vice versa. By this analogy, there is no reason why Delaunay should imply the dihedral angle criterion and vice versa.

Our examples also point out another weakness of combining FE and the Delaunay criterion: If the Delaunay tetrahedralization is not unique FE gives different results depending on the choice of tetrahedralization.

The finite volume schemes, however, only rely on the Voronoi boxes. In degenerate cases the result does not depend on the choice of tetrahedralization.

In this respect the dihedral angle criterion cannot achieve for FE what Delaunay achieves for FV. There may be several or no tetrahedralizations which fulfill the dihedral angle criterion and they will produce different solutions.

3.7 Discussion

3.7.1 The Abstract Viewpoint

Stemming from the equivalence of FE and FV in two dimensions there is a widely spread belief that this equivalence is also valid in higher dimensions, in other words that finite elements can be reduced to some kind of finite volumes and vice versa. However FE and FV are different with respect to the heuristical basis on which they are derived. Finite elements are a very general and flexible approach for which a sophisticated mathematical theory exists. On the other hand, there are finite volume schemes which are motivated more physically. Usually, the latter employ a conservation law or balance equations for control volumes using an integral theorem. [26] compares finite element and finite volume schemes using concepts from algebraic topology and the theory of differential forms. It explains why finite elements and finite volumes are different on a fundamental level and why "the charge brought against FE of reducing all to nodes must be reconsidered" [26].

In the special case of the Laplace operator it is still possible to interpret FE as a finite volume scheme in three dimensions, but in contrast to the two-dimensional case the corresponding finite volume scheme is based on gravity boxes instead of the Voronoi boxes [19].

3.7.2 Practical Strategies

In the attempt to avoid numerical instabilities the most important strategic decision is the proper choice of discretization. With respect to diffusion problems the decision is an easy one: use a variant of finite volumes. Many meshing tools construct their basic meshes relying on the Delaunay criterion, then possibly doing some kind of quality improvement. In any case, many available meshers are Delaunay-based. Finite

elements on a conventional Delaunay mesh however can be a disaster and are much more vulnerable and sensitive to the meshing quality.

If one wants or has to use a finite element solver a practical meshing strategy will generally try to avoid extremely obtuse (dihedral) angles and badly shaped elements without too much concern on the Delaunay property and without a technique to enforce the dihedral angle criterion directly. Existing meshing techniques often try to avoid any obtuse dihedral angles. This is not necessary if techniques can be developed to generate finite element meshes which satisfy the dihedral angle criterion. However such a technique remains open to further research.

In many practical cases one cannot rely on a very good quality of the FE mesh. Then additional strategies are pursued: e.g., mesh refinement combined with a time step reduction. According to standard finite element theory, the discretized solution (using backwards Euler) will converge to the exact solution if meshing granularity and time step size tend to zero. The main obstacle to make successful use of this property is the lack of a smart refinement strategy. There is no way to exclude global anisotropic effects as in Fig. 20. In cases like this getting rid of negative concentrations by *h*-refinement is not feasible.

Alternative strategies like the use of higher order shape functions (*p*-refinement) or a simplistic cutting off of negative concentrations are even less promising from a theoretical as well as from an empirical point of view.

3.7.3 Nonlinear Case

In the linear case the emergence of negative concentrations can be simply considered as an annoyance as long as the precision is high enough. In the nonlinear case the consequences of insufficient meshing quality are much more serious: Equation (15) is then solved by a Newton method. Exemplary simulations reveal that negative transmissibilities cause a deterioration of the convergence of the Newton iteration. For a physical explanation see [18].

The negative concentrations are particularly severe in diffusion problems for semiconductor process simulation, because in typical applications the concentration varies in many orders of magnitude within a small area. If the Newton iteration does not converge the time step is usually reduced. This can lead to convergence, but has no diminishing effect on the emerging negative concentrations. Therefore appropriate meshing quality is of utmost importance for the solution of nonlinear transient problems with high concentration gradients like, e.g., the pair diffusion model [27].

3.8 Resume

We presented a case study on the interplay between meshing and discretization in diffusion simulation. Finding meshing algorithms specially tuned for the discretization in use is a strong challenge to the TCAD community. From a mathematical point of view finite element schemes are often easier to analyze than finite volume schemes for the same problem. However with regard to easy fulfillment of the corresponding meshing requirements finite volumes are the superior discretization. Progress in the development of robust PDE solvers can only be achieved by a point of view which regards discretization and meshing not as two distinct tasks but as one problem with an analytic and a more algorithmic part. One instance for a solution is the perfect interplay between the finite volume discretization and Delaunay meshes. This symmetry is broken when finite elements are combined with the Delaunay criterion and it is restored only incompletely when Delaunay is replaced by the dihedral angle criterion.

3.8 Resume

Based on a vast series of numerical experiments conducted using AMIGOS and theoretical investigations we advocate the use of finite volume schemes in three-dimensional diffusion modeling.

4 Two-Dimensional Simulation of Ferroelectric Materials

4.1 Introduction

Recent development of ferroelectric devices has lead to two-dimensional and compound device designs. Even devices considered to be simple like a finger structure with a common ground plate lead to effects such as e. g. crosstalk which cannot be handled by a one-dimensional model, but are of fundamental interest. A side from this also the frequency dependence of the materials has to be taken into consideration as increasing clock frequencies lead into a regime where the frequency dependence of basic material parameters like coercive field and remanent polarization can no longer be neglected. At high frequencies, the hysteresis widens and the coercive field increases, which is of fundamental interest for the extraction of parameters for write and read cycles like applied voltage or pulse length.

4.2 Modeling

The basic goal of our approach is to set up a tool which is able to reproduce the macroscopic behavior of the device by calculating current, voltage and charge at the contacts correctly. Simulation of domains and impurities is far from trivial and needs device data like the impurity distribution, which is usually not available and furthermore specific for a singular device. According to this, the resulting domain structure differs even for devices with identical geometry and identical contact quantities. For our approach we set up the ferroelectric material as a homogeneous cluster of identical dipoles, each of them showing the macroscopic hysteresis properties. This results in a model which allows the two-dimensional analysis of ferroelectric materials, by introducing hysteresis to the polarization and solving the Poisson equation.

4.2.1 Two-Dimensional Model

In order to allow simulation of rotational effects the one-dimensional Preisach hysteresis model had to be generalized [28]. The remanent polarization components in non field directions are taken into account, respecting the fact that there is an upper limit to the number of dipoles as well.

4.2.2 Hysteresis Model

MINIMOS-NT offers a rigorous approach to treat the static hysteresis properties [28][29] of ferroelectric materials, which was recently extended to the exact calculation of subcycles.

Using the box integration method, the third Maxwell equation

$$\operatorname{div} \overline{D} = \rho \tag{32}$$

is solved. To bring in hysteresis, we separate the electric displacement into a linear and a nonlinear part

$$\vec{D} = \epsilon \cdot \vec{E} + \vec{P}.$$
(33)

The nonlinear part \vec{P} holds the hysteresis and is modeled by

$$P = k \cdot f(E \pm E_c, k) + P_{\text{off}}.$$
(34)



Figure 28: Simulated hysteresis including multiple subcycles

The parameters k and P_{off} are necessary for the simulation of the subcycles of the hysteresis, the function f is the shape function for the subcycles, E_c is the coercive field.

By now two different types of shape functions are implemented in the simulator, the tanh and the arctan function. The implementation for the tanh shaped function is

$$P = k \cdot P_{\text{sat}} \cdot \tanh(w \cdot (E \pm E_c)) + P_{\text{off}}.$$
(35)

 P_{sat} is the saturation polarization. w is a shape parameter and the same for each locus curve. This function is a good approach for the material properties of PZT(Pb(Zr, Ti)O_3).

$$P = \frac{2}{\pi} \cdot k \cdot P_{\text{sat}} \cdot \arctan(2 \cdot (E \pm E_c) \cdot \frac{k}{w}) + P_{\text{off}}.$$
(36)

is the implementation for the $\arctan shape$ function. Again, w is the shape parameter. The $\arctan function$ covers the physical properties of $SBT(SrBi_2Ta_2O_9)$ in a very accurate way. A drawback of this method is that the parameters of the locus curves have to be calculated numerically. This leads on one hand to a slight increase of computation time, on the other hand to some complications with regard to the numerical solution of the problems.

Using these subcycles the whole history of the ferroelectric material is simulated. The necessary parameters are calculated according to Preisach hysteresis [30]. This allows the simulation of the following effects:

- Locus curves hit last turning point: This allows the simulation of closed subcycles
- Memory wipe out: A turning point erases all information of previous smaller turning points

A complete set of subcycles is plotted in Fig. 28, showing the simulation results for a planar capacitor.

4.2.3 Transient Model

According to the concept of our device simulator MINIMOS-NT we tried to find an analytic model based on differential equations instead of an approach based on statistical physics [31] in order to model the transient properties.

We extended a common approach [32] for the frequency dependence of linear dielectric materials. We start with the static, nonlinear equation

$$P = f(E(t)). \tag{37}$$

Following our approach we add a transient term to the electric field

$$E(t) = E_{\text{stat}} + \tau_{ef} \cdot \frac{dE}{dt}$$
(38)

where E_{stat} is the static component of the electric field and τ a material dependent time constant. The actual electric field is calculated and can be entered into (Eq. 37), thus forming the first term for the transient equation

$$P_{\rm ef} = f(E(t)). \tag{39}$$

Basically, this terms shifts the hysteresis curves and increases the coercive field. Still following the approach for linear materials, we add a transient term stemming from the change of the polarization

$$P_{\rm pol} = -\tau_{\rm pol} \cdot \frac{dP}{dt}.$$
(40)

Again τ_{pol} is a time constant. Aside from increasing the coercive field as well, this term flattens the hysteresis. Experimental data shows that these two terms can be fitted into the physical properties in a limited range of frequencies only. In order to improve this,

$$P = P_{\rm pol} + P_{\rm nonlin} \tag{41}$$

a third term, representing the nonlinearity of the material, was added,

$$P_{\text{nonlin}} = c \cdot k_{\text{nonlin}} \cdot (P - P_{\text{ef}}) \cdot \frac{dE(t)}{dt}.$$
(42)

This term allows also a physical interpretation as it increases with the offset between the polarization component stemming from the electric field and the actual polarization. k_{nonlin} is a material dependent constant.

Both transient equations (Eq. 38) and (Eq. 41) are discretized with a forward Euler scheme, which garanties a reasonable stability.

4.3 Examples

With our model it is now possible to analyze arbitrary devices and to extract material parameters.

26

4.3 Examples

4.3.1 Extraction of Equivalent Parameters of a Finger Structure

The finger structure, outlined is the basic structure used for high integrated memory cells. To calculate the basic hysteresis we simulated the area marked in Fig. 29. Fig. 30 shows the simulated Q–V characteristic of of this two-dimensional device and compares it to the result of the simple 1d-structure with the same width. It already shows properties and effects that exceed the one-dimensional case. As a result of the well known edge effect of the electric field, the electric field in this areas will reach the coercive field even for small contact voltages. This leads to an area of polarization reversal (Fig. 31) and to a decrease of the coercive field of the device.



Figure 29: Cross section of a finger structure and simulated area



Figure 30: 'One-dimensional' capacitor versus finger structure

By the help of this simulation results it is possible to extract new hysteresis parameters for a one-dimensional device which allow the accurate simulation of this two-dimensional structure. The resulting Q–V characteristics of this calibration are outlined in Fig. 32. This ability of the simulator is very useful as it reduces the afford substantially, and allows the usage of a compact model. This way this opens the door to an exact circuit simulation.



Figure 31: Polarization reversal near the edge of the contact



Figure 32: Comparison of the transfer characteristics of a finger structure and the 'one-dimensional' capacitor with fitted hysteresis parameters



Figure 33: Charge and current response of a voltage jump

4.3.2 Switching of a capacitor

With our model, the analysis of ferroelectric memory cells for arbitrary variation of the contact voltage is now possible. Fig. 33 shows the time depending current and charge when a voltage jump is applied to a capacitor, Fig. 34 for a triangular signal with an included delay.

Especially in the first of these two figures the behavior of the ferroelectric material leads to a significant difference compared with a linear dielectric. The dipole relaxation does not follow an exponential function as might be expected and the maximum current does not appear immediately after the voltage step. As a consequence of equation (Eq. 38), the electric field cannot change immediately inside the device, so the whole hysteresis curve has to be swept during the relaxation period, which causes the unexpected smoothness of the charge characteristics and the shift of the maximum current to the right.

As outlined above, our model allows the simulation of ferroelectric materials in a wide range of frequencies.



Figure 34: Charge and current response of a transient simulation



Figure 35: Coercive voltage as a function of frequency and peak voltage

From there, frequency dependent material parameters like the coercive voltage (Fig. 35), or the remanent polarization can be easily obtained. These can be used to emulate the frequency dependence with the static model, which might be useful if the applied frequency stays in the same range.

5 Inductance Calculation in Interconnect Structures

5.1 Introduction

With increasing packaging density and raising signal frequencies inductance effects in interconnect structures gain importance for the electrical behavior of circuits. The largest TCAD commercial vendors present a wide range of solutions for interconnect simulations. These tools (e.g. [33, 34]) have userfriendly and task-oriented interfaces, but still lack some of the features we have incorporated. Our package SAP (Smart Analysis Programs [35]) offers the calculation of, e.g., partial self- and mutualinductances [36] of interconnect structures. The inductance calculation is based on the computation of the magnetostatic field energy, whereby first the current distributions of the interconnect structures is calculated by means of the finite element method.

5.2 Physical approach

The influence of the skin effect is neglected, thus results are valid as long as the skin depth $\delta = 1/\sqrt{\mu\gamma\omega}$ is large compared to the diameters of the interconnect structures. μ denotes the magnetic permeability, γ the electrical conductivity and ω the angular frequency. As example: $\delta = 2.6 \,\mu m$ for copper at 1 GHz.

The physical details on which our method is based and their numerically consequences are sketched in the following. Because of the universal validity of $\nabla \cdot \mathbf{B} = 0$, we introduce the magnetic vector potential according to $\mathbf{B} = \nabla \times \mathbf{A}$. By choosing the Coulomb gauge $\nabla \cdot \mathbf{A} = 0$, we get

$$-\nabla^2 \mathbf{A} = \mu \mathbf{J} \,. \tag{43}$$

A particular solution of (43) is

$$\mathbf{A}(\mathbf{r}) = \frac{\mu}{4\pi} \int_{V'} \frac{\mathbf{J}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} dV', \qquad (44)$$

where V' is the volume of all conductors. Instead of evaluating the magnetic vector potential in (44) and calculating the energy of the magnetostatic field with

$$W = \frac{1}{2} \int_{V} \mathbf{J}(\mathbf{r}) \cdot \mathbf{A}(\mathbf{r}) \, dV, \tag{45}$$

we compute the energy directly with the Neumann formula [37]:

$$W = \frac{\mu}{8\pi} \int_{V} \int_{V'} \frac{\mathbf{J}(\mathbf{r}) \cdot \mathbf{J}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} dV' dV.$$
(46)

Pursuing the energy concept leads to the 6-fold integral

$$L_{ik} = \frac{\mu}{4\pi} \frac{1}{I_i I_k} \int_{V_i} \int_{V'_k} \frac{\mathbf{J}_i(\mathbf{r}) \cdot \mathbf{J}_k(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} dV' dV, \qquad (47)$$

where \mathbf{r}, \mathbf{r}' denotes locations and V_i respectively V'_k the conductive segments, and I_i, I_k are the total currents through these segments. This equation is handled differently, depending whether self-inductances (i = k) or mutual-inductances $(i \neq k)$ are calculated. Note, that (47) can be simplified by assuming a uniform current density in the conductors. This relates the inductances only to the geometry. However, this results in closed form expressions only for elementary shapes of geometries. Hence, for complex structures with tetrahedral elements the evaluation of the 6-fold integral has to be done numerically.

5.3 Implementation

5.3.1 The Program Package SAP

The program package SAP consists of 7 modules. Fig. 36 shows the main tools of the package SAP and displays the data-flow. The simulation is performed with the module STAP (Smart Thermal Analysis Programs [38]) which uses the finite element method to solve the Laplace equation for domains of conducting materials. We obtain the potential distribution by solving the linear equation system with a preconditioned conjugate gradient solver. By applying Ohm's law to the derivative of the electrostatic potential the distribution of the electric current density is obtained. The layout of the interconnect structure can be imported



Figure 36: The Smart Analysis Programs

from CIF or GDSII files, or can be created interactively with a graphical layout editor [39]. The geometry can be defined either directly from the layout by specifying layer thicknesses, or by a rigorous topography simulation [40, 41]. Furthermore, the program package includes three preprocessors, one for two-dimensional applications (CUTGRID [42]) the other for three-dimensional applications. The meshing strategy of DELINK [43] follows the concept of Delaunay methods. The preprocessed surface description provides the initial front. The preprocessor LAYGRID [44] allows a layer-based input of the simulation geometry with boundary conditions of either Neumann or Dirichlet type specified on the borders of each simulation subdomain. We use tetrahedral grid elements with quadratic shape functions for our layerbased grid generation method. A global grid level refinement is also available as well as a possibility of refinement for an area of interest.

Two postprocessors complete the program package, whereby the visualization tool SV is based on VTK [45]. The second postprocessor FEMPOST can be used to verify the grid quality, and for the visualization of severe distributions (e.g. electric potential, temperature, current density).

5.3.2 Mutual Inductances

With the knowledge of the current density we can calculate the magnetostatic field energy to extract the partial inductances. Fig. 37 shows a simple test example and Table 1 the comparison of the results with values received by the formula of Grover [37] as well known reference.

d (cm)	computed (nH)	Grover (nH)
0.1 cm	41.6	41.9
0.3 cm	23.3	23.5
0.5 cm	16.3	16.5
0.7 cm	12.6	12.7

Table 1: Mutual inductance of two conductors (radius is 0.2 cm and the length is 10 cm) with distance d between their centers



Figure 37: Potential distribution of two parallel conductors with circular cross section

The mutual-inductance is calculated by rewriting the integrations as summations over each element of the conductors *i* and *k*. With quadratic shape functions ten nodes per element are used for taking the average of the current density over the element. This is possible, because the term $|\mathbf{r} - \mathbf{r}'|$ is nearly constant if the element size is small compared to the distance between the conductors. Then the term $|\mathbf{r} - \mathbf{r}'|$ can be approximated by the distance between the centers of the elements.

5.3.3 Self Inductances

For the computation of self inductances more advanced strategies have to be applied. Fig. 38 shows the current density of an spiral inductor, which has following dimensions: area: 226 x 226 μm , metal width = 18 μm , wire-spacing = 10 μm and the height of the spiral inductor amounts 2.7 μm . The analysis of this example took 27 minutes on an Digital Alpha workstation (DEC600/333 MHz), resulting 2.05 nH for the self inductance. The calculation of the self inductances demand special formulae with certain integration points, published by Stroud [46], who presented various integration formulae which are applicable for various n-simplexes (e.g. the unit triangle, the unit tetrahedron) as integration region. To extract the self-inductances (47) has to be transformed to the unit tetrahedron:

$$L_{ii} = \frac{\mu}{4\pi I_i I_i} \cdot \int\limits_{\upsilon \in V_i} \int\limits_{\upsilon' \in V'_i} \mathbf{J}_i \left(\mathbf{r} \left(\xi, \eta, \zeta \right) \right) \cdot \mathbf{J}_i \left(\mathbf{r}' \left(\xi', \eta', \zeta' \right) \right) \cdot \frac{\det J \det J'}{\left| \mathbf{r}(\xi, \eta, \zeta) - \mathbf{r}'(\xi', \eta', \zeta') \right|} \, d\upsilon' d\upsilon \quad (48)$$



Figure 38: Current density distribution in a spiral inductor

 V_i respectively V'_i denote the conductive segments of the ith electrical subsystem, ξ , η , ζ are the local coordinates and detJ, detJ' are the transformation determinants, which are not a function of the local coordinates. The kernel of (48) is significant for the behavior of the integral equation, especially if the locations \mathbf{r}, \mathbf{r}' lay in the same tetrahedron it is challenging to compute the integral equation numerically. Thus two strategies are used: For the summations over all different tetrahedrons two formulae with certain integration points are used. According to [47] we utilize the integration formula of the form

$$\int \cdots \int f(x_1, \cdots, x_n) dx_1 \cdots dx_n = \sum_{i=1}^N A_i f(p_i)$$
(49)

where S_n is an n-dimensional simplex. The A_i are constants and the $p_i = (p_{i1}, p_{i2}, \dots, p_{in})$ are points in an n-dimensional space. These points can be obtained from Table I [47] by permutation of the four coordinates

$$\begin{array}{rl} \nu_1 &= 0.0948 \\ \nu_2 &= \nu_1 \\ \nu_3 &= 0.2412 \\ \nu_4 &= 0.5690, \end{array}$$

e.g. $p_{i1} = (\nu_1, \nu_2, \nu_3)$. The second formula applicable to this case is found in [48], formula IV, with the set of points (0,0,0; 1), resp. (1/3,1/3,1/3; 0). This notation denotes the set of points consisting of (0,0,0) and all permutations with 1. These two sets of points are weighted with two different, positive constants. For the interpolation of the current density inside each element the quadratic shape functions are used.

For all summations over identical tetrahedrons an analytic integration in the third coordinate (ζ, ζ') is done, before the two formulae of Stroud [46] for the unit triangle are utilized, namely formula T_n 2-1, with the set (0.16,0.16; 0.66) and formula T_n 3-6 with the set (0.109,0.232; 0.659), both of them weighted with positive constants.

References

- H. Kosina, M. Nedjalkov, and S. Selberherr. A Monte Carlo Method for Small Signal Analysis of the Boltzmann Equation. J.Appl.Phys., 87(99):4308–4314, 2000.
- [2] M. Nedjalkov, H. Kosina, and S. Selberherr. Monte-Carlo Method for Direct Computation of the Small Signal Kinetic Coefficients. In SISPAD'99 [49], pp 155–158.
- [3] E. Starikov and P. Shiktorov. New Approach to Calculation of the Differential mobility Spectrum of Hot Carriers: Direct modeling of the Gradient of the Distribution Function by the Monte Carlo Method. Sov. Phys. Semicond., 22(1):45–48, 1988.
- [4] Y. Pozhela, E. Starikov, and P. Shiktorov. Dynamic NDM at Transit Time Resonance in n-InP. Semicond.Sci.Technol., 7:B386–B389, 1992.
- [5] C. Jacoboni and P. Lugli. *The Monte Carlo Method for Semiconductor Device Simulation*. Springer, Wien-New York, 1989.
- [6] T.Kuhn and F.Rossi. Monte Carlo Simulation of Ultrafast Processes in Photoexcited Semiconductors: Coherent and Incoherent Dynamics. *Physical Review B*, 46(12):7496–7514, 1992.
- [7] J.Schilp, T.Kuhn, and G.Mahler. Electron-Phonon Quantum Kinetics in Pulse-Excited Semiconductors: Memory and Renormalization Effects. *Physical Review B*, 50(8):5435–5447, 1994.
- [8] M.Nedjalkov and I.Dimov. Statistical Modelling of Pulse Excited Electron Quantum Kinetics in One Band Semiconductor. *Mathematics and Computers in Simulations*, 47, 1998.
- [9] J.Barker and D.Ferry. Self-Scattering Path-Variable Formulation of High Field, Time-Dependent Quantum Kinetic Equations for Semiconductor Transport in the Finite-Collision-Duration Regime. *Physical Review Letters*, 42(26):1779–1781, 1979.
- [10] R. Brunetti, C. Jacoboni, and F. Rossi. Quantum theory of transient transport in semiconductors: A Monte Carlo approach. *Physical Review B*, 39(15):10781–10790, 1989.
- [11] C. Jacoboni, P. Poli, and L. Rota. A new Monte Carlo Technique for the Solution of the Boltzmann Transport Equation. *Solid-State Electron.*, 31(3/4):5523–526, 1988.
- [12] M. Nedjalkov, I. Dimov, and H. Haug. Numerical Studies of the Markovian Limit of the Quantum Kinetics with Phonon Scattering. *Phys.stat.sol.(b)*, 209:109–121, 1998.
- [13] G. Hobler, L. Pelaz, and C.S. Rafferty. Continuum Treatment of Spatial Correlation in Damage Annealing. Nuclear Instruments and Methods in Physics Research, 153(1-4):172–176, 1999.
- [14] Semiconductor Industry Association. The National Technology Roadmap for Semiconductors, 1999.
- [15] M. Protter and H. Weinberger. *Maximum principles in differential equations*. Springer, New York, 1984.
- [16] C. Pao. Nonlinear Parabolic and Elliptic Equations. Plenum Press, New York, 1992.
- [17] R. Bapat and T. Raghaven. *Nonnegative Matrices and Applications*. Cambridge University Press, Cambridge, 1997.
- [18] P. Forsyth. A Control Volume Finite Element Approach to NAPL Groundwater Contamination. *SIAM J.Sci.Stat.Comput.*, 12(5):1029–1057, 1991.

- [19] M. Putti and Ch. Cordes. Finite Element Approximation of the Diffusion Operator on Tetrahedra. *SIAM J.Sci.Comput.*, 19(4):1154–1168, 1998.
- [20] R.E. Bank and D.J. Rose. Some Error Estimates for the Box Method. *SIAM J.Numer.Anal.*, 24(4):777–787, 1987.
- [21] F.W. Letniowski. Three-Dimensional Delaunay Triangulations for Finite Element Approximations to a Second-Order Diffusion Operator. SIAM J.Sci.Stat.Comput., 13(3):765–770, 1992.
- [22] M.Radi, E. Leitner, and S. Selberherr S. AMIGOS: Analytical Model Interface & General Object-Oriented Solver. *IEEE Trans. Semiconductor Technology Modeling and Simulation*, (2), 1999.
- [23] T. Ikeda. *Maximum Principle in Finite Element Models for Convection-Diffusion Phenomena*. North Holland, Amsterdam, 1983.
- [24] J. Xu and L. Zikatanov. A Monotone Finite Element Scheme for Convection-Diffusion Equations. *Mathematics of Computation*, 68(228):1429–1446, 1999.
- [25] P. Fleischmann, B. Haindl, R. Kosik, and S. Selberherr. Investigation of a Mesh Criterion for Three-Dimensional Finite Element Diffusion Simulation. In SISPAD'99 [49], pp 71–74.
- [26] C. Mattiussi. An Analysis of Finite Volume, Finite Element, and Finite Difference Methods Using Some Concepts from Algebraic Topology. J.Comput. Phys., 133(2):289–309, 1997.
- [27] W.B. Richardson, G.F. Carey, and B.J. Mulvaney. Modeling Phosphorus Diffusion in Three Dimensions. *IEEE Trans. Computer-Aided Design*, 11(4):487–496, 1992.
- [28] K. Dragosits and S. Selberherr. Numerical Aspects of the Simulation of Two-Dimensional Ferroelectric Hysteresis. In *Proc. 2nd Intl. Conf. on Modeling and Simulation of Microsystems*, pp 309–312, San Juan, Puerto Rico, USA, 1999.
- [29] K. Dragosits, M. Knaipp, and S. Selberherr. Two-Dimensional Simulation of Ferroelectric Memory Cells. *Journal of the Korean Physical Society*, 35:104–106, July 1999.
- [30] F.Preisach. Über die magnetische Nachwirkung. Zeitschrift für Physik, 94:277–302, 1935.
- [31] M. Takeo, M. Azuma, H. Hirano, K. Asari, N. Moriwaki, T. Otsuki, and K. Tatsuuma. SrBi₂Ta₂O₉ Thin Film Capacitor Model Including Polarization Reversal Response for Nanosecond Range Circuit Simulation of Ferroelectric Nonvolatile Memory. In *Proc.Intl.Electron Devices Meeting*, pp 621– 624, 1997.
- [32] G. Fasching. Werkstoffe für die Elektrotechnik. Springer, Wien, 1987. 2. Auflage.
- [33] Technology Modeling Associates (now part of Avant!). *RAPHAEL Reference Manual*. Sunnyvale, California, 1997.
- [34] TEMPEST Manual. Silvaco International, Santa Clara, California, 1997.
- [35] R. Sabelka, R. Martins, and S. Selberherr. Accurate Layout-Based Interconnect Analysis. In Meyer and Biesemans [50], pp 336–339.
- [36] A. E. Ruehli. Inductance Calculations in a Complex Integrated Circuit Environment. *IBM J.Res.Dev.*, 16(1):470–481, 1972.
- [37] F. W. Grover. *Inductance Calculations: Working Formulas and Tables*. D. Van Nostrand Company, New York, 1946.

- [38] R. Sabelka and S. Selberherr. SAP A Program Package for Three-Dimensional Interconnect Simulation. In Proc. Intl. Interconnect Technology Conference, pp 250–252, Burlingame, California, 1998.
- [39] R. Martins and S. Selberherr. Layout Data in TCAD Frameworks. In *Modelling and Simulation*, pp 1122–1126. Society for Computer Simulation International, 1996.
- [40] R. Martins, W. Pyka, R. Sabelka, and S. Selberherr. High-Precision Interconnect Analysis. IEEE Trans. Computer-Aided Design, 17(11):1148–1159, 1998.
- [41] W. Pyka, R. Martins, and S. Selberherr. Efficient Algorithms for Three-Dimensional Etching and Deposition Simulation. In Meyer and Biesemans [50], pp 16–19.
- [42] Robert Bauer and Siegfried Selberherr. Preconditioned CG-Solvers and Finite Element Grids. In Proc. CCIM, volume 2, Breckenridge, USA, 1994.
- [43] P. Fleischmann, W. Pyka, and S. Selberherr. Mesh Generation for Application in Technology CAD. *IEICE Trans.Electron.*, E82-C(6):937–947, 1999.
- [44] P. Fleischmann, R. Sabelka, A. Stach, R. Strasser, and S. Selberherr. Grid Generation for Three-Dimensional Process and Device Simulation. In *Simulation of Semiconductor Processes and Devices*, pp 161–166, Tokyo, Japan, 1996. Business Center for Academic Societies Japan.
- [45] W. Schroeder, K. Martin, and B. Lorensen. The Visualization Toolkit: An Object-Oriented Approach to 3D Graphics. Prentice-Hall, 1996.
- [46] A. H. Stroud. Approximate Calculation of Multiple Integrals. Prentice-Hall, Englewood Cliffs, N.J., 1971.
- [47] A. H. Stroud. Some Approximate Integration Formulas of Degree 3 for an n-Dimensional Simplex. *Numer.Math.*, 9:38–45, 1966.
- [48] A. H. Stroud. Approximate Integration Formulas of Degree 3 for Simplexes. 18:590–597, 1964.
- [49] Proc. Simulation of Semiconductor Processes and Devices, Kyoto, Japan, 1999.
- [50] K. De Meyer and S. Biesemans, editors. *Proc. Simulation of Semiconductor Processes and Devices*, Leuven, Belgium, 1998. Springer.