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Modelling and Simulation of Power Devices for High-Voltage Integrated Circuits

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Abstract. Process and device simulators turned out to be important tools in the design of high-voltage integrated circuits and in the development of their technology. The main goal of this project was the improvement of the device simulator `WIAS-TeSCA` in order to simulate different power devices in high-voltage integrated circuits developed by the industrial partner. Some simulation results are presented. Furthermore, we discuss some aspects of the mathematics of relevant model equations which device and process simulations are based on.

1 Introduction

In the computer aided design of high-voltage *Integrated Circuits* (ICs) and in the development of their technology process and device simulation programmes turned out to be important tools. Challenges of new technologies and devices require a permanent discussion of underlying physical models, the mathematical analysis of related model equations, as well as the improvement of simulation codes. The main goal of this project was the extension of the device simulator `WIAS-TeSCA` [Gaj] by a self-consistent coupling of the van Roosbroeck system with a heat flow equation since thermal and thermoelectric effects play some rôle in power devices.
The industrial partner of the project is the company *alpha microelectronics gmbh* Frankfurt (Oder). The company develops and produces application-specific ICs for high-voltage applications (e.g. driver ICs for coils, motors and relays). The basis for all high-voltage ICs is a proprietary *500 V dielectric isolated MOS technology* [Kno] which uses thick-film bonded silicon-on-insulator wafers with dielectric trench isolation.
Different power devices in the high-voltage ICs of the company were used as test structures for the development and application of `WIAS-TeSCA`. Here we present simulation results for a *dielectric isolated, double Diffused Metal Oxide Semiconductor Transistor* (DMOST). Furthermore, we discuss some aspects of the mathematics of relevant model equations which device and process simulations are based on.

2 Process Simulation

The simulation of the technological process of manufacturing semiconductor devices is used to develop such processes and to optimize them with respect to the device geometry and doping, for instance. We applied the process simulator `DIOS-ISE` [Str]. In Fig. 1 the simulated cross-section of a typical axisymmetric DMOST test structure with two gate contacts is shown. For the grid generation a compromise between accuracy and effort was reached. The defaults of the diffusion parameters could mostly be used; only the redistribution of dopants during oxidation needed some changes. For this structure

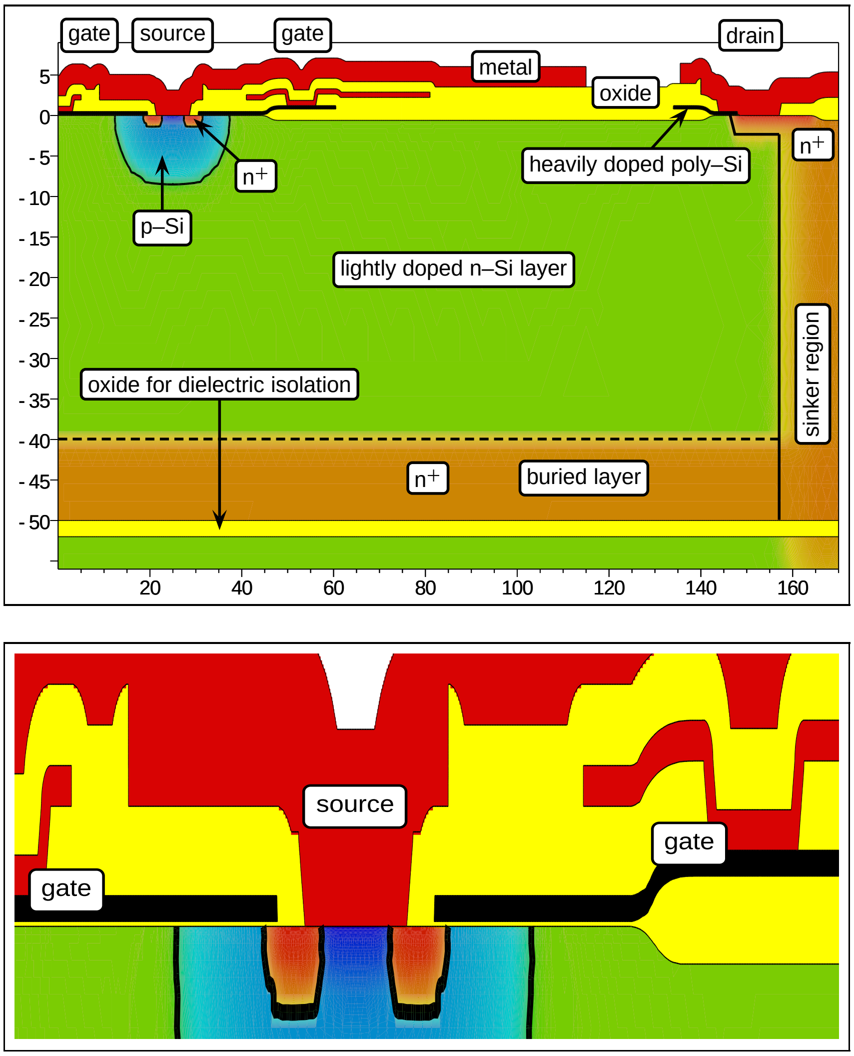


Fig. 1. `DIOS-ISE` simulation result for the DMOST: cross-section (top, the unit of length is micron, the axis of rotation lies on the left hand side, Si – silicon) and detail of the source and gate contact regions (bottom)

the thickness of the silicon layer and the doping concentrations (in the silicon layer, buried layer, sinker region) were varied to get different devices. Process simulation results are taken as input for subsequent device simulations.

3 Device Simulation

As mentioned in the introduction the device simulator `WIAS-TeSCA` was improved in order to be able to simulate power devices successfully. Now we shortly discuss some simulation results.
The aim of device simulation is to evaluate the electrical behaviour of the device. Often stationary current-voltage characteristics are required showing e.g. the drain current versus the drain(-source) voltage with the gate(-source) voltage as a parameter (see Figs. 2, 3, 4). Important device properties are derived from these characteristics which have to be optimized. The on-resistance is given by the reciprocal slope in the origin of the characteristics. The breakdown voltage characterizes the electrical breakdown of the device caused by avalanche generation of carriers due to impact ionization in high field regions and resulting in a drastic increase of the current. The knowledge of regions of high electric field strength, and thus also of high avalanche generation rate, is very useful for the designer to optimize the breakdown voltage. Finally, inhomogeneities of the temperature caused by large power densities at higher drain voltages should also influence the device behaviour since decisive physical parameters depend strongly on the temperature.
One important task for the simulation was the investigation of the influence of different dielectric isolated substrates on the device behaviour. In order to demonstrate the effect of the electric field we chose two DMOST structures as in Fig. 1, one has a buried layer, the other has not. For estimating the

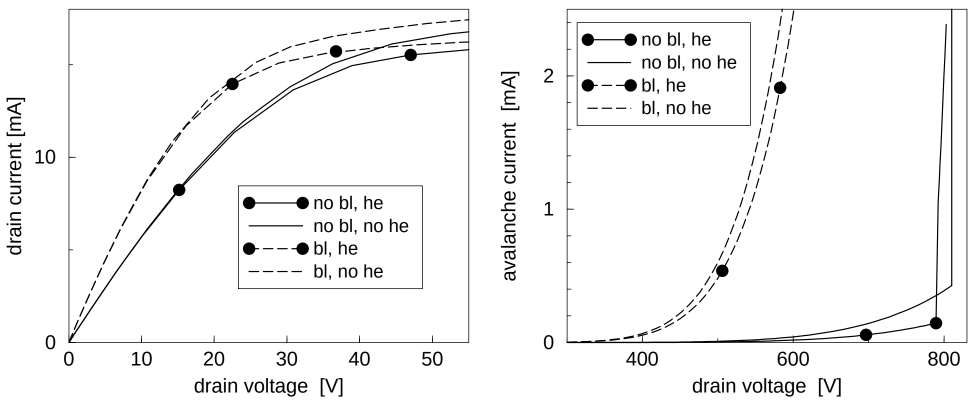
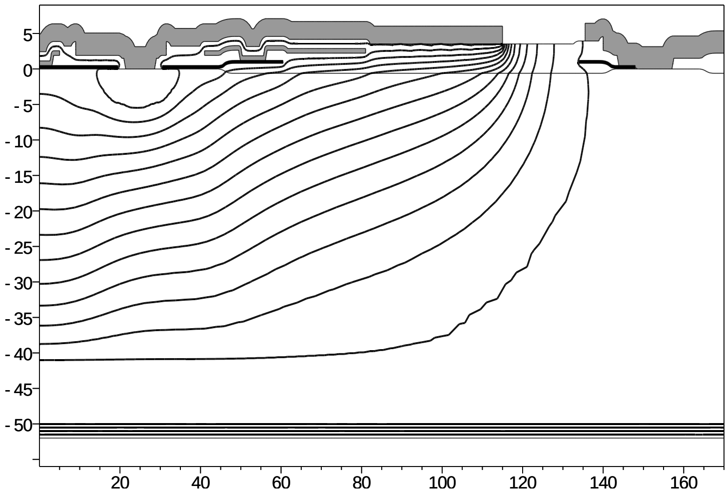


Fig. 2. `WIAS-TeSCA` simulation results for the DMOST: current-voltage characteristics at low drain voltages (left, bl – buried layer, he – heat flow equation) and avalanche generation current at high drain voltages (right)

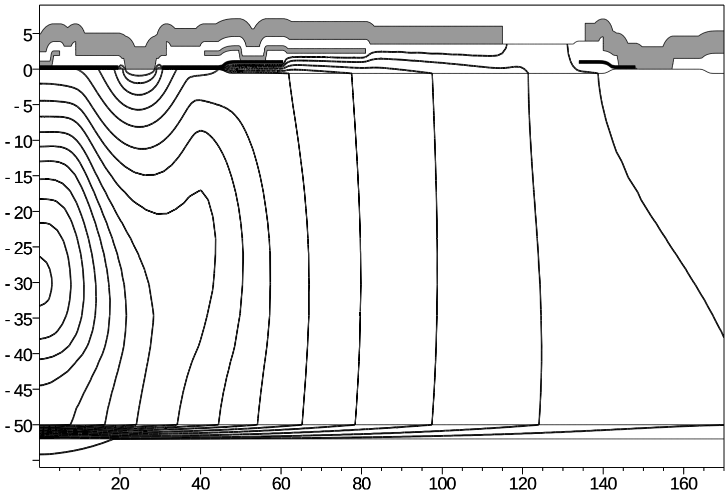
Electrostatic potential

Isolines for a drain voltage of 600 V



Temperature

Isolines for a drain voltage of 600 V (the maximal device temperature lies on the axis of rotation)



Current-voltage characteristics

Solid line: simulation with heat flow equation (in some points the maximal device temperature $T_{\max}$ [K] is indicated)

Dashed line: simulation for fixed temperature $T = 300\,\mathrm{K}$

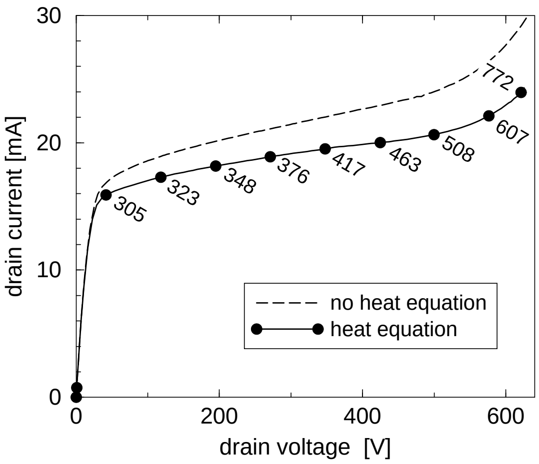
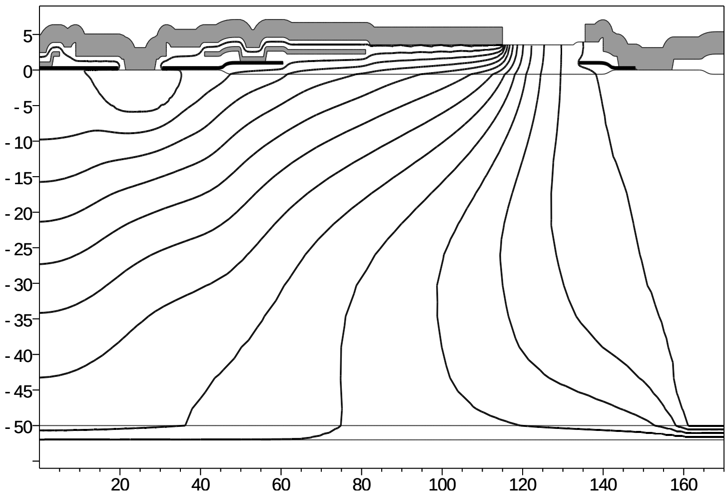


Fig. 3. Simulation results for the DMOST with a $10\,\mu$m thick buried layer

Electrostatic potential

Isolines for a drain voltage of 600 V



Current-voltage characteristics

Solid line: simulation with heat flow equation (in some points the maximal device temperature $T_{\max}$ [K] is indicated)

Dashed line: simulation for fixed temperature $T = 300\,\mathrm{K}$

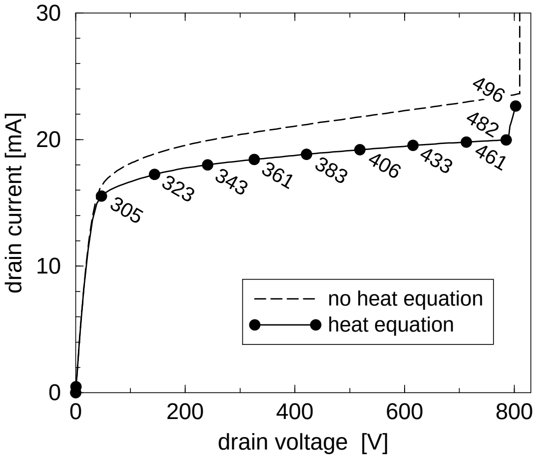


Fig. 4. Simulation results for the DMOST without buried layer

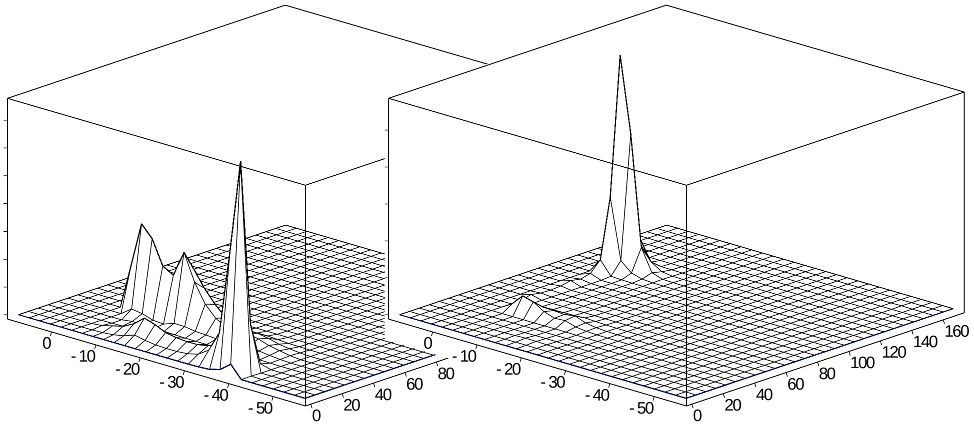


Fig. 5. Avalanche generation rate near the breakdown voltage for the DMOST with (left) and without (right) buried layer

effect of inhomogeneities of the temperature all simulations were done with and without using the heat flow equation. On all electrical contacts and on the bottom of the slice (more precisely, in a depth of 100μm) the temperature was fixed at 300 K while on the other parts of the boundary homogeneous Neumann conditions were posed.
Figure 2 shows current-voltage characteristics which are used for the determination of the on-resistance and breakdown voltage. Isolines of the electrostatic potential as well as the current-voltage characteristics at 10 V gate voltage are given in Fig. 3 for the structure with a buried layer and in Fig. 4 for the structure without a buried layer. Figure 3 shows also isolines of the temperature. For the structure without a buried layer isolines of the temperature look similarly, but the values of the temperature are much lower. The electrostatic potential differs clearly in both devices such that the regions of high avalanche generation rate are also quite different, see Fig. 5.

4 Device Modelling

Simulations with `WIAS-TeSCA` are based on some energy model that extents the basic drift-diffusion model [Gaj] by a heat flow equation. There is a large variety of energy models (see e.g. [Kel] and references therein). Our approach can be found in [AGH]. Starting with a generally accepted expression for the density of the free energy and applying only first principles like the entropy maximum principle and the principle of local equilibrium a system of evolution equations is derived for different variants of energy models (including the Boltzmann or Fermi-Dirac statistics, non-parabolic band structures, electron-hole scattering models, the kinetics of deep traps, and hot carrier effects). Particular attention is paid to include the electrostatic potential self-consistently.
Here we describe a simple version of such a model. We start with state equations of the form

$$n_i = \overline{n}_i(T)\,\mathrm{e}^{(\zeta_i - q_i\psi)/T}, \quad \overline{n}_i(T) = [m_i(T)T]^{3/2}\,\mathrm{e}^{q_i E_i(T)/T}, \quad i = 1,2 \ ,$$

$$u = u(n_1, n_2, T) = c_{\mathrm{L}}T + \sum_{i=1}^{2} n_i T^2 \frac{\partial \log \overline{n}_i}{\partial T}(T) \ ,$$

$$s = s(n_1, n_2, T) = c_{\mathrm{L}} \log T + \sum_{i=1}^{2} n_i P_i(n_i, T) \ , \quad P_i = 1 + T\,\frac{\partial \log \overline{n}_i}{\partial T} - \log \frac{n_i}{\overline{n}_i}$$

where n_1 is the electron density, $q_1 = -1$, n_2 is the hole density, $q_2 = 1$, ζ_i are the electrochemical potentials, ψ is the electrostatic potential, T is the lattice temperature, m_i and E_i are the effective masses (up to a constant factor) and energy band edges, u denotes the density of the internal energy, s the density of entropy, c_L is the heat capacity of the lattice, and P_i are the thermoelectric powers.

The potential ψ fulfills the Poisson equation

$$-\nabla \cdot (\varepsilon \nabla \psi) = f - n_1 + n_2 \tag{1}$$

where ε is the dielectric permittivity, f is a given doping profile and does not depend on time. A mixed boundary condition is used,

$$\psi = \psi^D \text{ on } \Gamma_D \ , \quad \varepsilon \frac{\partial \psi}{\partial \nu} + \tau(\psi - \psi^N) = 0 \text{ on } \Gamma_N \tag{2}$$

where Γ denotes the boundary of the domain Ω occupied by the device, Γ_D and Γ_N are disjoint, relatively open parts of Γ with $\mathrm{mes}\,(\Gamma \setminus (\Gamma_D \cup \Gamma_N)) = 0$. The particle fluxes j_i and the *reduced* heat flux j_q are assumed to be given by

$$j_i = -\sigma_i(n_1, n_2, T)\,(\nabla \zeta_i + P_i \nabla T) \ , \quad j_q = -\lambda(n_1, n_2, T)\,\nabla T$$

with conductivities σ_i, $\lambda > 0$. A first form of the system of evolution equations consists of two continuity equations and a heat flow equation,

$$\frac{\partial n_i}{\partial t} + \nabla \cdot j_i = -R \ , \quad c(n_1, n_2, T)\,\frac{\partial T}{\partial t} + \nabla \cdot j_q = H \tag{3}$$

with the net recombination rate

$$R = \rho(n_1, n_2, T)\,(\mathrm{e}^{(\zeta_1 + \zeta_2)/T} - 1) \ , \quad \rho > 0 \ ,$$

the heat capacity $c = \partial u / \partial T > 0$, and the heat generation rate

$$H = \sum_{i=1}^{2} \left[\frac{|j_i|^2}{\sigma_i} - T\,\nabla P_i \cdot j_i + [\zeta_i + (P_i - 1)T]\,R - T\,\nabla \cdot j_i \right]$$

representing especially the Joule, Thomson and Peltier heating rates as well as the recombination heat (cf. [Alb,Kel,Wac]). This form of the evolution equations was the starting point for the implementation of the energy model in `WIAS-TeSCA`. The heat flow equation can be replaced by other balance equations, too.
Firstly, defining the energy flux $j_u = j_q + \sum_{i=1}^{2} (\zeta_i + P_i T) j_i$, the energy balance equation

$$\frac{\partial u}{\partial t} + \nabla \cdot j_u = -\psi\,\nabla \cdot (j_1 - j_2)$$

is obtained. If we introduce the total energy density $\widetilde{u} = u + \frac{\varepsilon}{2} |\nabla \psi|^2$ and the total energy flux $j_{\widetilde{u}} = j_u + \psi\,\partial D / \partial t$, $D = -\varepsilon \nabla \psi$, then the last equation becomes a conservation law,

$$\frac{\partial \widetilde{u}}{\partial t} + \nabla \cdot j_{\widetilde{u}} = 0 \ . \tag{4}$$

Concerning this result our approach differs from those given in [BS,Kel,Wac].

Secondly, defining the entropy flux $j_s = j_q/T + \sum_{i=1}^{2} P_i j_i$, the entropy balance equation

$$\frac{\partial s}{\partial t} + \nabla \cdot j_s = \sigma \tag{5}$$

is derived where σ denotes the entropy production rate,

$$\begin{aligned}
T\sigma &= \sum_{i=1}^{2} \frac{1}{\sigma_i}|j_i|^2 + \frac{1}{\lambda T}|j_q|^2 + \sigma_R = \sum_{i=1}^{2} \sigma_i \,|\nabla\zeta_i + P_i \nabla T|^2 + \frac{\lambda}{T}\,|\nabla T|^2 + \sigma_R \\
&= -T \sum_{i=1}^{2} j_i \cdot \nabla \frac{\zeta_i}{T} + T\, j_u \cdot \nabla \frac{1}{T} + \sigma_R \\
&= -\sum_{i=1}^{2} j_i \cdot \nabla\zeta_i - j_s \cdot \nabla T + \sigma_R, \quad \sigma_R = \rho\,(\mathrm{e}^{(\zeta_1+\zeta_2)/T} - 1)(\zeta_1 + \zeta_2) \ .
\end{aligned}$$

Obviously $\sigma \geq 0$ holds, and $\sigma = 0$ if and only if $\nabla\zeta_i = 0$, $\nabla T = 0$, $\zeta_1 + \zeta_2 = 0$ (thermodynamic equilibrium). The Onsager relations are valid if either the fluxes (j_1, j_2, j_u) and the generalized forces $(\nabla[\zeta_1/T], \nabla[\zeta_2/T], -\nabla[1/T])$, or the fluxes (j_1, j_2, j_s) and the generalized forces $(\nabla\zeta_1, \nabla\zeta_2, \nabla T)$ are used.

The equations (4), (5) reflect the First Law and Second Law of Thermodynamics in differential form. In order to get their integral form we introduce the functionals of total energy and total entropy,

$$U(n_1, n_2, T) = \int_{\Omega} \left[\frac{\varepsilon}{2}\,|\nabla\psi|^2 + u(n_1, n_2, T)\right] \mathrm{d}x + \int_{\Gamma_N} \frac{\tau}{2}\,\psi^2 \,\mathrm{d}\Gamma \ ,$$

$$S(n_1, n_2, T) = \int_{\Omega} s(n_1, n_2, T)\,\mathrm{d}x \ .$$

Assuming that the system is thermodynamically closed ($j_i \cdot \nu = 0$, $j_q \cdot \nu = 0$ on Γ) we obtain that

$$\frac{\mathrm{d}U}{\mathrm{d}t} = \int_{\Gamma_D} \varepsilon\,\nabla \frac{\partial\psi}{\partial t} \cdot \nu\,\psi^D \,\mathrm{d}\Gamma + \int_{\Gamma_N} \tau\,\psi\,\frac{\partial\psi^N}{\partial t}\,\mathrm{d}\Gamma \ , \quad \frac{\mathrm{d}S}{\mathrm{d}t} = \int_{\Omega} \sigma\,\mathrm{d}x$$

along any solution of (3), (1), (2). The second equation shows that the negative total entropy $-S$ is a Lyapunov function of the evolution system. The first equation implies that the total energy is preserved if $\psi^D = 0$ and ψ^N does not depend on time.

These important properties of the evolution system remain valid for the corresponding discrete system what has been achieved by using sophisticated discretization schemes with respect to time and space coordinates. Thus the energy model implemented in `WIAS-TeSCA` turns out to be well posed from the thermodynamic point of view. From the mathematical point of view the evolution system is very complicated, and there are known only few results, at least under realistic assumptions on the state equations and kinetic coefficients. For the stationary case in [Gri] new existence and uniqueness results are obtained using the Implicit Function Theorem and properties of linear elliptic operators in a suitable scale of Sobolev-Campanato spaces.

5 Process Modelling

One of the main process steps in manufacturing semiconductor devices is the redistribution of dopants connected with or followed after the doping. In order to simulate this process, different models have been developed. Nowadays so called pair diffusion models are preferred [Dun,GH,Höf,Str]. They consist in a set of reaction-diffusion equations for a lot of electrically charged species $X_1, \ldots, X_m$ (dopants, point defects, dopant–defect pairs, see Fig. 6). The kinetics of electrons and holes is assumed to be very fast. Then the electrochemical potential of the electrons does not depend on the spatial coordinates, and for determining their chemical potential, denoted by ψ again, a boundary value problem for a nonlinear Poisson equation is obtained,

$$-\nabla \cdot (\varepsilon \nabla \psi) = f + e(\psi) + \sum_{i=1}^{m} n_i \, q_i(\psi) \ , \ \nabla \psi \cdot \nu \,|_\Gamma = 0 \ . \qquad (6)$$

Here f, $e(\psi)$, n_i and $q_i(\psi)$ denote a fixed background doping, the charge density of electrons and holes, the density of the species X_i and its charge number depending on ψ, respectively.
The initial boundary value problem for the reaction-diffusion system is

$$\frac{\partial n_i}{\partial t} + \nabla \cdot j_i = - \sum_{(\alpha,\beta) \in \mathcal{R}} (\alpha_i - \beta_i) \, R_{\alpha\beta} \ , \quad j_i \cdot \nu \,|_\Gamma = 0 \ , \quad n_i(0) = N_i \quad (7)$$

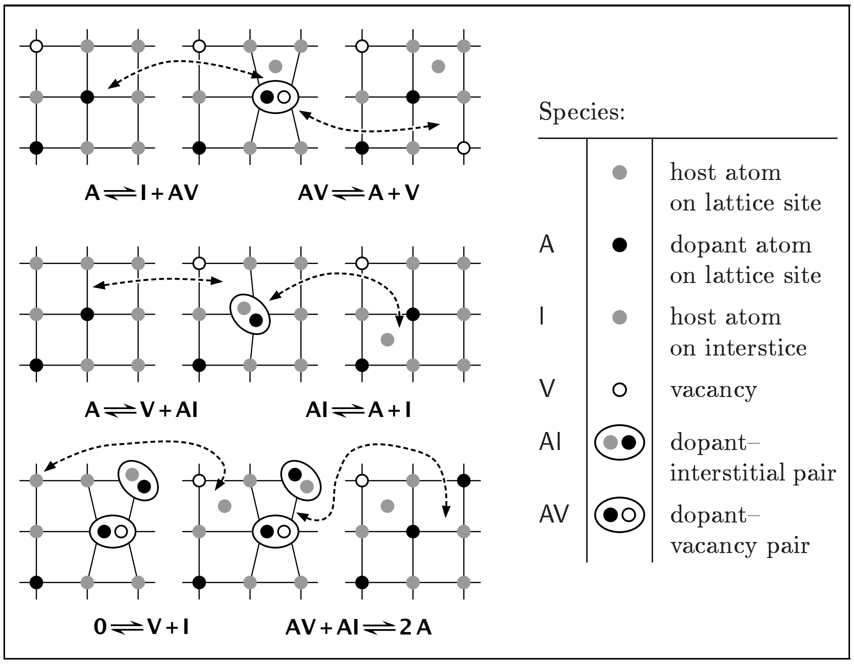


Fig. 6. Species and reactions in a variant of pair diffusion models

where the particle fluxes j_i and reaction rates $R_{\alpha\beta}$ are given by

$$j_i = -D_i(\psi)\ [\nabla n_i + n_i\, q_i(\psi)\nabla\psi]\ ,$$

$$R_{\alpha\beta} = k_{\alpha\beta}(\psi)\left[\prod_{i=1}^m a_i^{\alpha_i} - \prod_{i=1}^m a_i^{\beta_i}\right],\ a_i = \frac{n_i}{p_i(\psi)}\ ,\ p_i(\psi) = \overline{n}_i\, \mathrm{e}^{-\int_0^\psi q_i(s)\,\mathrm{d}s}\ .$$

Here the vector $(\alpha,\beta) = (\alpha_1,\dots,\alpha_m,\beta_1,\dots,\beta_m)$ represents the stoichiometric numbers of mass action type reactions of the form

$$\alpha_1 \mathrm{X}_1 + \cdots + \alpha_m \mathrm{X}_m \rightleftharpoons \beta_1 \mathrm{X}_1 + \cdots + \beta_m \mathrm{X}_m\ ,\quad (\alpha,\beta)\in\mathcal{R}\ .$$

The kinetic coefficients $D_i(\psi)$ and $k_{\alpha\beta}(\psi)$ are generally positive (only for the dopants often $D_i = 0$ is proposed). Finally, $\overline{n}_i$ is a positive reference density, N_i is the non-negative initial density of the i-th species.
If the charge numbers do not depend on ψ we arrive at a model that we have studied in a previous project [HGGR]. In the more general situation considered now the mathematical investigation starts from thermodynamic principles, again. Since we deal only with isothermal processes, the energy functional that has to be chosen is the total free energy [HG],

$$F(n) = \int_\Omega \left\{ \frac{\varepsilon}{2}|\nabla\psi|^2 \mathrm{d}x + \int_0^\psi [e(s) - e(\psi)]\,\mathrm{d}s + \sum_{i=1}^m n_i \int_0^\psi [q_i(s) - q_i(\psi)]\,\mathrm{d}s \right.$$
$$\left. + \sum_{i=1}^m \left[n_i\left(\ln\frac{n_i}{\overline{n}_i} - 1\right) + \overline{n}_i \right] \right\}\mathrm{d}x$$

where ψ is the solution of (6) for prescribed densities $n = (n_1,\dots,n_m)$. Under some assumptions concerning the initial values and the structure of the underlying reaction system we have proved in [HG] the following results. The time derivative of the free energy fulfills the inequality

$$\frac{\mathrm{d}F}{\mathrm{d}t} \le -\int_\Omega d\,\mathrm{d}x$$

along any solution of (7), (6), d is a lower estimate of the dissipation rate,

$$d = \sum_{i=1}^m 4\,D_i(\psi)\,p_i(\psi)\ \left|\nabla\sqrt{a_i}\right|^2 + \sum_{(\alpha,\beta)\in\mathcal{R}} 2\,k_{\alpha\beta}(\psi)\left|\prod_{i=1}^m \sqrt{a_i}^{\,\alpha_i} - \prod_{i=1}^m \sqrt{a_i}^{\,\beta_i}\right|^2 .$$

Since $d \ge 0$ the free energy is a Lyapunov function of the evolution system. Moreover, there exists a steady state n^* (with corresponding potential ψ^*) which is uniquely determined in the class

$$\left\{ n\colon \int_\Omega (n - N)\,\mathrm{d}x \in \operatorname{span}\{\alpha - \beta\colon (\alpha,\beta)\in\mathcal{R}\} \right\}.$$

The difference $F(n) - F(n^*)$ decays exponentially to zero if the time tends to infinity. Based on these properties of the free energy further a priori estimates and existence results can be derived. First results are obtained in [MGHP].

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