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# EINDHOVEN UNIVERSITY OF TECHNOLOGY Department of Mathematics and Computing Science

# RANA 92-06 March 1992 AN EXPONENTIAL FITTING SCHEME FOR THE ELECTROTHERMAL DEVICE EQUATIONS, SPECIFICALLY FOR THE SIMULATION OF AVALANCHE GENERATION by J.H.M. ten Thije Boonkkamp W.H.A. Schilders



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# An exponential fitting scheme for the electrothermal device equations, specifically for the simulation of avalanche generation

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#### Abstract

An extension of the Scharfetter-Gummel discretisation scheme is presented which is designed especially for the electrothermal semiconductor device equations including avalanche generation terms. The scheme makes explicit use of the exponential character of solutions, and reduces to the standard Scharfetter-Gummel scheme in the isothermal non-avalanche case.

# 1 Introduction

Over the last few decades, the size of semiconductor device structures has decreased dramatically, and this process is still continuing. Because of this, the need for mathematical modelling of such structures is rapidly growing. So far, the most widely used model for describing the behaviour of semiconductor devices is the drift-diffusion model. This model consists of Poisson's equation for the electrostatic potential and continuity equations for holes and electrons. Simulations using this model have been shown to agree well with experiments in many cases. Improved models for the parameters in the model, such as carrier mobilities, bandgap narrowing and recombination (cf. [1]), effectively extend the applicability of the model. Although much attention is paid to extended models ([2, 3]), such as the hydrodynamic model, the conventional drift-diffusion model is still adequate for the simulation of many devices.

The simulation of the behaviour of semiconductor devices using the drift-diffusion model offers substantial difficulties, arising in all phases of the numerical solution procedure ([4]). Therefore, special methods have been developed over the past decade to solve the associated problems in a robust and efficient manner. Research in this area has led to special discretisation methods (the well-known Scharfetter-Gummel scheme [5], mixed finite element methods [6]), special non-linear solution techniques ([7, 8]) and the use of state-of-the-art techniques for the solution of large sparse linear systems ([4, 9]). In addition, customised techniques have been developed for special models. When avalanche generation is included in the model, the character of the equations changes dramatically, and the methods developed need adjusting. In [10], an extended Scharfetter-Gummel scheme is presented which makes use of the exponential character of the problem.

In this paper we consider a simple extension of the drift-diffusion model, in which the lattice temperature is introduced as an additional unknown. Thus, carriers are still assumed to be in thermal equilibrium, but the overall temperature of the device may vary. The effect of this extension is reflected in the model by an extra equation for the lattice temperature, and by different expressions for the current densities. The latter will not only contain terms relating to drift and diffusion, but also a term due to temperature gradients. In addition, we assume that the recombination/generation term contains the mechanism of avalanche generation. We will derive special discretisation methods for this model, which take into account the varying temperature as well as the exponential behaviour of the current densities. We will only elaborate on the discretisation of the current relations, since the other equations involved do not provide any significant problems when using the box method.

An outline of the paper is as follows. In the next section we first give an overview of the equations which constitute the model, followed by a description of the parameters used. Section 3 contains the derivation of the extensions of the Scharfetter-Gummel scheme for 1-dimensional problems, both in the isothermal and the non-isothermal cases. The former is, in fact, a summary of the material presented previously in [10], and is used to explain the main ideas; the latter then discusses the application of these ideas to the case of variable lattice temperature. In Section 4, the discrete schemes derived are elaborated further. Especially for the non-isothermal cases, difficulties occur in the approximation of integrals involved; remedies for this are described. Section 5 then discusses the extension of the 1-dimensional methods to the case of 2-d rectangular grids; although the basic idea of this extension is similar to that of the traditional Scharfetter-Gummel scheme, again specific difficulties are encountered. These are described in this section, as well as their treatment. The paper is concluded with a summary of the most important aspects of the methods presented.

### 2 The electrothermal device equations

The set of partial differential equations describing the stationary, electrothermal behaviour of semiconductor devices reads [11]

(2.1) 
$$\nabla \cdot (\varepsilon \mathbf{E}) = \rho, \quad \rho = q(p - n + D),$$
  
(2.2a)  $\nabla \cdot \mathbf{J}_n = -\alpha_n |\mathbf{J}_n| - \alpha_p |\mathbf{J}_p| + qR,$   
(2.2b)  $\nabla \cdot \mathbf{J}_p = \alpha_n |\mathbf{J}_n| + \alpha_p |\mathbf{J}_p| - qR,$   
(2.3)  $\nabla \cdot (\kappa \nabla T) = -H.$ 

Equation (2.1) is the Poisson equation, (2.2a) and (2.2b) are the electron and hole continuity equation, respectively, and (2.3) is the heat conduction equation. In these equations, the electric field  $\mathbf{E}$  and the electron and hole current densities  $\mathbf{J}_n$  and  $\mathbf{J}_p$  are given by

(2.4) 
$$\mathbf{E} = -\nabla \psi$$
,  
(2.5a)  $\mathbf{J}_n = q(\mu_n n \mathbf{E} + D_n \nabla n + n D_n^T \nabla T)$ ,  
(2.5b)  $\mathbf{J}_p = q(\mu_p p \mathbf{E} - D_p \nabla p - p D_p^T \nabla T)$ .

Equations (2.5a) and (2.5b) are referred to as the electron and hole current relation, respectively. The basic variables in (2.1)-(2.5) are the electrostatic potential  $\psi$ , the electron and hole concentrations n and p, and the (absolute) device temperature T. Physical parameters in the above equations are the space charge density  $\rho$ , the doping profile D, the electron and hole ionisation rates  $\alpha_n$  and  $\alpha_p$ , the recombination/generation rate R, the thermal conductivity  $\kappa$ , the heat generation rate H, the electron and hole mobilities  $\mu_n$  and  $\mu_p$ , the diffusion coefficients  $D_n$  and  $D_p$  and the thermal diffusion coefficients  $D_n^T$  and  $D_p^T$  (see Appendix). In addition, the system (2.1)-(2.5) contains two constants, viz. the permittivity  $\varepsilon$  and the elementary charge q.

Here, we briefly discuss some models for the physical parameters. For a more detailed discussion, see e.g. [1, 11]. The doping profile D is defined as the net concentration of all ionised impurities, i.e.

 $(2.6) \quad D=N_D-N_A,$ 

where  $N_D$  and  $N_A$  are the concentrations of ionised donors and acceptors, respectively. Here we assume that all impurity atoms are singly ionised. Closely related to D is the total impurity concentration N, defined by

$$(2.7) \quad N = N_D + N_A.$$

Most of the following physical parameters are a function of N.

At low electric fields, the drift velocity of the charge carriers is linearly proportional to the electric field, and the proportionality factors are called the carrier mobilities  $\mu_c(c=n,p)$ . The mobilities  $\mu_c$  are determined by various scattering mechanisms, such as for instance lattice scattering or impurity scattering. At high electric fields however, the drift velocities saturate due to carrier heating. This effect is accounted for by fielddependent carrier mobilities. In general,  $\mu_c = \mu_c(N, T, \mathbf{E}, n, p)$ . A comprehensive discussion can be found in [11]. Here we only present a typical example

(2.8) 
$$\mu_c = \frac{\mu_{c,LI}}{1 + \frac{\mu_{c,LI}|\mathbf{E}|}{v_{c,rat}}} \quad (c = n, p),$$

where  $\mu_{c,LI}$  is the mobility due to lattice scattering and impurity scattering only, and where  $v_{c,sat}$  is the so-called saturation velocity. In this paper we assume that the diffusion coefficients  $D_n, D_p$  are related to the mobilities  $\mu_n, \mu_p$  by the Einstein relation

(2.9) 
$$D_c = U_T \mu_c \ (c = n, p), \quad U_T = \frac{kT}{q},$$

where  $U_T$  is the thermal voltage and k is the Boltzmann constant. Furthermore, we assume the following relation between the diffusion coefficients  $D_n, D_p$  and the thermal diffusion coefficients  $D_n^T, D_p^T$  ([12])

(2.10) 
$$\frac{D_c^T}{D_c} = \frac{r+1}{T}.$$

In (2.10) r is a constant depending on the dominant scattering type. If for instance lattice scattering is dominant then  $r = -\frac{1}{2}$ . However, if impurity scattering dominates then  $r = \frac{3}{2}$ .

The recombination/generation rate R is the number of electron-hole pairs which recombine or are generated per unit volume and per unit time. When recombination prevails, R > 0, and otherwise, when generation prevails, R < 0. Note that in (2.2a) and (2.2b) we have explicitly split off the avalanche generation term

(2.11a) 
$$R_{II} = -\frac{1}{q} (\alpha_n \mid \mathbf{J}_n \mid +\alpha_p \mid \mathbf{J}_p \mid),$$

since it plays such a dominant role in the following. Avalanche generation is also often called impact ionisation. The most commonly used models for R are the Shockley-Read-Hall function

(2.11b) 
$$R_{SRH} = \frac{np - n_{int}^2}{\tau_p(n + n_{int}) + \tau_n(p + n_{int})},$$

and the Auger function

(2.11c) 
$$R_{Au} = (C_{n,Au}n + C_{p,Au}p)(np - n_{int}^2).$$

In (2.11b), (2.11c)  $\tau_n$  and  $\tau_p$  are the electron and hole lifetimes, respectively, and  $n_{int}$  is the intrinsic carrier concentration. The total recombination rate (excluding avalanche generation) is the sum of  $R_{SRH}$  and  $R_{Au}$ . Avalanche generation is only of importance at high electric fields. In fact, in this case  $R_{II}$  completely dominates the other recombination terms. A typical expression for the ionisation rates  $\alpha_c$  is

(2.12) 
$$\alpha_c = \alpha_{c,\infty}(T) \exp\left(-\frac{E_{c,crit}(T)}{|E_c|}\right), (c=n,p),$$

with  $E_c = \mathbf{E} \cdot \mathbf{J}_c / |\mathbf{J}_c|$ . In other words,  $E_c$  is the projection of  $\mathbf{E}$  in the direction of  $\mathbf{J}_c$ .

In this paper we assume that  $n_{int}$  is a constant, i.e. we ignore bandgap narrowing, because it is not of importance in the derivation of the exponential fitting scheme. However, extension of this scheme for a variable intrinsic carrier concentration  $n_{int}$  is straightforward.

A model for the thermal conductivity is ([11])

(2.13) 
$$\kappa(T) = (a + bT + cT^2)^{-1}$$
.

Finally, consider the heat generation rate H, which is the heat generated in the device per unit volume and per unit time. A thorough description of H can be found in [13]. Here we only present the so-called Joule heating term

(2.14) 
$$H = \frac{1}{q} \left( \frac{|\mathbf{J}_n|^2}{\mu_n n} + \frac{|\mathbf{J}_p|^2}{\mu_p p} \right),$$

which is the heat generated due to the flow of carriers through an electric field. Note that H > 0, i.e. heat is generated in the device and not consumed.

The equations (2.1)-(2.5) have to be solved on a domain  $\Omega$ , which consists of the semiconductor material, but which may also contain regions of a different type, such

as oxide, plastic or metal. Only the heat conduction equation (2.3) has to be solved on the whole domain. The electrical device equations (2.1),(2.2),(2.4) and (2.5) only hold in the semiconductor material, and in the oxide region only the Poisson equation has to be solved with space charge density  $\rho = 0$ . The set of differential equations (2.1)-(2.5) has to be completed with appropriate boundary conditions.

For the derivation of the discretisation scheme it is convenient to introduce the quasi-Fermi potentials  $\varphi_n, \varphi_p$  and the Slotboom variables u, v. These variables are defined in [14, 15]

(2.15) 
$$\varphi_n = \psi - U_T \ln\left(\frac{n}{n_{int}}\right), \varphi_p = \psi + U_T \ln\left(\frac{p}{n_{int}}\right),$$

and

(2.16) 
$$u = e^{-\varphi_n/U_T}, v = e^{\varphi_p/U_T}.$$

In the isothermal case, i.e. T is constant, the current relations (2.5) can be rewritten in terms of these variables as follows

(2.17a) 
$$\mathbf{J}_n = -q\mu_n n \nabla \varphi_n,$$
  
(2.17b)  $\mathbf{J}_p = -q\mu_p p \nabla \varphi_p,$ 

or

(2.18a) 
$$\mathbf{J}_n = q D_n n_{int} e^{\psi/U_T} \nabla u,$$
  
(2.18b)  $\mathbf{J}_p = -q D_p n_{int} e^{-\psi/U_T} \nabla v.$ 

Clearly, the quasi-Fermi potentials act in this case as the driving force for the current densities. In the non-isothermal case, the current relations (2.17) and (2.18) have to be supplemented with an extra term proportional to  $\nabla T$ .

# **3** Derivation of the 1-dimensional exponential fitting scheme

#### 3.1 The isothermal case

In this section we describe an exponential fitting scheme for the continuity equations and the current relations, originally developed in [10]. The 1-dimensional continuity equations read

(3.1a) 
$$J'_{n} = -\alpha_{n} | J_{n} | -\alpha_{p} | J_{p} | +qR,$$
  
(3.1b)  $J'_{p} = \alpha_{n} | J_{n} | +\alpha_{p} | J_{p} | -qR.$ 

The current relations are, expressed in terms of the quasi-Fermi potentials or the Slotboom variables:

(3.2a) 
$$J_n = -q\mu_n n \varphi'_n = q D_n n_{int} e^{\psi/U_T} u',$$
  
(3.2b)  $J_p = -q\mu_p p \varphi'_p = -q D_p n_{int} e^{-\psi/U_T} v'.$ 

There are two difficulties associated with the continuity equations (3.1). Firstly, these equations are intrinsically coupled and secondly, they are nonlinear in  $J_n$  and  $J_p$ . However, this nonlinearity can be overcome as follows. Define  $s_n = sign(J_n), s_p = sign(J_p)$ , then  $|J_n| = s_n J_n$  and  $|J_p| = s_p J_p$ , and from equation (3.2) it is obvious that  $s_n = -sign(\varphi'_n)$  and  $s_p = -sign(\varphi'_p)$ . Therefore, the continuity equations can now be written as

$$(3.3a) \quad \mathbf{J}' = A\mathbf{J} + q\mathbf{R},$$

with

(3.3b) 
$$\mathbf{J} = \begin{pmatrix} J_n \\ J_p \end{pmatrix}, A = \begin{pmatrix} -\beta_n & -\beta_p \\ \beta_n & \beta_p \end{pmatrix}, \mathbf{R} = \begin{pmatrix} R \\ -R \end{pmatrix},$$

where  $\beta_n = s_n \alpha_n$  and  $\beta_p = s_p \alpha_p$ . Thus (3.3a) may be considered as a linear system with a non-constant coefficient matrix A.

For space discretisation, the domain  $\Omega$  is covered with a non-uniform mesh. Assuming a piecewise constant electric field E between neighbouring mesh points  $x_i$  and  $x_{i+1}$ , A is a piecewise constant matrix. In particular for  $x \in [x_i, x_{i+1}]$ ,  $A = A_{i+1/2}$ , see Fig. 1. Then, the exact solution of (3.3a) subject to the boundary condition  $J(x_{i+1/2}) = J_{i+1/2}$  is

(3.4) 
$$\mathbf{J}(x) = e^{(x-x_{i+1/2})A_{i+1/2}} \mathbf{J}_{i+1/2} + q \int_{x_{i+1/2}}^{x} e^{(x-s)A_{i+1/2}} \mathbf{R}(s) ds,$$

clearly demonstrating an exponential behaviour of J(x) due to the avalanche generation term.

Equation (3.3a) is discretised using the box method (finite volume technique [16]). Therefore, consider the box  $B_i = [x_{i-1/2}, x_{i+1/2}]$  around mesh point  $x_i$ . Integration of (3.3a) over the box  $B_i$  gives

(3.5) 
$$\mathbf{J}_{i+1/2} - \mathbf{J}_{i-1/2} = \int_{x_{i-1/2}}^{x_i} A_{i-1/2} \mathbf{J} dx + \int_{x_i}^{x_{i+1/2}} A_{i+1/2} \mathbf{J} dx + q \int_{x_{i-1/2}}^{x_{i+1/2}} \mathbf{R} dx$$

Consider the second integral. Assume that for  $x \in [x_i, x_{i+1}]$ , J(x) satisfies

(3.6) 
$$\mathbf{J}(x) = e^{(x-x_{i+1/2})A_{i+1/2}} \mathbf{J}_{i+1/2}.$$

This assumption is equivalent to the requirement that **J** satisfies the homogeneous equation  $\mathbf{J}' = A_{i+1/2}\mathbf{J}$ . Substitution of (3.6) in the second integral of (3.5) gives

(3.7) 
$$\int_{x_i}^{x_{i+1/2}} A_{i+1/2} \mathbf{J} dx = (I - e^{(x_i - x_{i+1/2})A_{i+1/2}}) \mathbf{J}_{i+1/2}.$$

The first integral in (3.5) can be computed in a similar way. The discrete continuity equation then reads

(3.8) 
$$e^{(x_i - x_{i-1/2})A_{i+1/2}} \mathbf{J}_{i+1/2} - e^{(x_i - x_{i-1/2})A_{i-1/2}} \mathbf{J}_{i-1/2} = qb_i \mathbf{R}_i,$$

where  $b_i = x_{i+1/2} - x_{i-1/2}$  is the size of box  $B_i$ . Note that the last integral in (3.5) is approximated by a simple midpoint rule. Also notice that for A = O (no avalanche generation), the original box scheme is obtained.

Now consider the current relations formulated in terms of the Slotboom variables. These equations can be written in vector form as follows

$$(3.9a) \quad \mathbf{J} = D\mathbf{u}',$$

with

(3.9b) 
$$\mathbf{u} = \begin{pmatrix} u \\ v \end{pmatrix}, D = q n_{int} \begin{pmatrix} D_n e^{\psi/U_T} & 0 \\ 0 & -D_p e^{-\psi/U_T} \end{pmatrix}$$

Substitution of (3.6) in (3.9a) and integration over  $[x_i, x_{i+1}]$  gives the following expression for  $J_{i+1/2}$ 

(3.10) 
$$\mathbf{J}_{i+1/2} = (\int_{x_i}^{x_{i+1}} D^{-1} e^{(x-x_{i+1/2})A_{i+1/2}} dx)^{-1} (\mathbf{u}_{i+1} - \mathbf{u}_i),$$

where  $\mathbf{u}_i = \mathbf{u}(x_i)$ , etc. Observe that the assumption about **J** is a straightforward generalisation of the assumption that **J** is constant for  $x \in [x_i, x_{i+1}]$  ( $\mathbf{J}' = 0$ ) made in the standard Scharfetter-Gummel scheme. For A = O (no avalanche generation), (3.10) reduces to the standard Scharfetter-Gummel scheme. The equations (3.8) and (3.10) are the discrete continuity equations and current relations, respectively. An elaboration of the scheme will be presented in Section 4.

#### 3.2 The non-isothermal case

Now we briefly discuss an extension of the exponential fitting scheme of the previous section, for the case of a variable device temperature. The main difficulty in this case is the additional term proportional to  $\nabla T$  in the current relations. Using the relations (2.9) and (2.10), the 1-dimensional current relations can be written as

(3.11a) 
$$J_n = qD_n(n' - n\psi'_n/U_T), \quad \psi_n = \psi - (r+1)U_T,$$
  
(3.11b)  $J_p = -qD_p(p' + p\psi'_p/U_T), \quad \psi_p = \psi + (r+1)U_T.$ 

In (3.11),  $\psi_n$  and  $\psi_p$  are modified potentials emanating from the  $\nabla \psi$  and  $\nabla T$  terms in the current relations. In the isothermal case we have  $\psi_n = \psi_p = \psi$ . Note that the thermal voltage  $U_T$  is not constant.

We like to write the current relations in a form similar to (3.2), so that we immediately can determine the sign (or direction) of  $J_n$  and  $J_p$ . Thus, consider the following representation for the current densities on the interval  $[x_i, x_{i+1}]$ 

(3.12a) 
$$J_n = q D_n e^{a_n} (n e^{-a_n})'$$
,  
(3.12b)  $J_p = -q D_p e^{-a_p} (p e^{a_p})'$ .

Then it is easy to show that the functions  $a_n(x)$  and  $a_p(x)$  are given by

(3.13a) 
$$a_n(x) = a_n(x_i) + \int_{x_i}^x \frac{\psi'_n(s)}{U_T(s)} ds,$$
  
(3.13b)  $a_p(x) = a_p(x_i) + \int_{x_i}^x \frac{\psi'_p(s)}{U_T(s)} ds,$ 

where the constants  $a_n(x_i)$  and  $a_p(x_i)$  can be chosen arbitrarily. Remark that in the isothermal case  $a_n = a_p = \psi/U_T$  (up to an additional constant), in accordance with (3.2). The current relations (3.12) can be rewritten in the following alternative ways. Define the variables  $\tilde{\varphi}_n, \tilde{\varphi}_p$  and  $\tilde{u}, \tilde{v}$  corresponding with respectively  $\varphi_n/U_T, \varphi_p/U_T$  and u, v, cf. (2.15) and (2.16),

(3.14) 
$$\tilde{\varphi_n} = a_n - \ln\left(\frac{n}{n_{int}}\right), \tilde{\varphi_p} = a_p + \ln\left(\frac{p}{n_{int}}\right),$$
  
(3.15)  $\tilde{u} = e^{-\tilde{\varphi_n}}, \tilde{v} = e^{\tilde{\varphi_p}}.$ 

Then, the current relations, expressed in these variables, read

$$\begin{array}{ll} (3.16a) & J_n = -q D_n n \tilde{\varphi}'_n = q D_n n_{int} e^{a_n} \tilde{u}', \\ (3.16b) & J_p = -q D_p p \tilde{\varphi}'_p = -q D_p n_{int} e^{-a_p} \tilde{v}'. \end{array}$$

Assume that the variables  $\tilde{\varphi}_n, \tilde{\varphi}_p$  are known, then the sign of  $J_n$  and  $J_p$  can be determined from (3.16). Henceforth, the derivation of the discretisation scheme is completely analogous to the isothermal case. Equation (3.8) is again the discrete continuity equation. The current relations (3.9) and the formula (3.10) for  $J_{i+1/2}$  also hold in the non-isothermal case, if the vector  $\mathbf{u} = (u, v)^T$  and the matrix D are replaced by respectively  $\tilde{\mathbf{u}} = (\tilde{u}, \tilde{v})^T$  and

$$(3.17) \quad D = qn_{int} \left( \begin{array}{cc} D_n e^{a_n} & 0 \\ 0 & -D_p e^{-a_p} \end{array} \right).$$

To complete the derivation of the exponential fitting scheme, we have to compute the functions  $a_n(x)$  and  $a_p(x)$ . These functions are defined per interval  $[x_i, x_{i+1}]$ . Let  $x \in [x_i, x_{i+1}]$  and assume that  $\psi$  and T are linear on this interval. The linearity assumption for  $\psi$  is in accordance with the previous assumption that E is constant on  $[x_i, x_{i+1}]$ . The functions  $a_n(x)$  and  $a_p(x)$  can be easily computed from (3.13), and we find

(3.18a) 
$$a_n(x) = a_n(x_i) - (E + (r+1)U'_T) \frac{x - x_i}{\overline{U}_T(x_i, x)},$$
  
(3.18b)  $a_p(x) = a_p(x_i) - (E - (r+1)U'_T) \frac{x - x_i}{\overline{U}_T(x_i, x)}.$ 

 $\bar{U}_T(x_i, x)$  is the harmonic average of  $U_T(s)$  on the interval  $[x_i, x]$ , defined by

(3.19) 
$$\bar{U}_T(x_i, x)^{-1} = \frac{1}{x - x_i} \int_{x_i}^x \frac{ds}{U_T(s)}.$$

Since  $U_T(s)$  is linear on  $[x_i, x]$ , the following expression for  $\overline{U}_T(x_i, x)$  is obtained

(3.20) 
$$\bar{U}_T(x_i, x) = \frac{U_T(x) - U_T(x_i)}{\ln U_T(x) - \ln U_T(x_i)}$$

Using Taylor expansion, one can easily see that in the isothermal case  $\bar{U}_T(x_i, x) = U_T$ , as is to be expected.

# 4 Elaboration of the scheme

The exponential fitting scheme consists of the discrete continuity equations (3.8) and the discrete current relations (3.10). In this section we further elaborate on these two equations. In particular, we discuss the computation of the matrix exponential  $e^{xA}$  and the current densities  $J_{i+1/2}$ , respectively.

Let A be a constant matrix. There are various ways to compute  $e^{xA}$ , see e.g. [17]. Since A is a  $2 \times 2$  matrix with eigenvalues 0 and  $\lambda = \beta_p - \beta_n$ , it is easy to show that

(4.1a) 
$$e^{xA} = I + \gamma(x)A$$
,

with

(4.1b) 
$$\gamma(x) = \begin{cases} \frac{1}{\lambda} (e^{\lambda x} - 1) & \text{if } \lambda \neq 0 \\ x & \text{if } \lambda = 0. \end{cases}$$

When we substitute this expression for  $e^{xA}$  in (3.8), the discrete continuity equations become

(4.2) 
$$(I + \gamma_{i+1/2}(x_i - x_{i+1/2})A_{i+1/2}) \mathbf{J}_{i+1/2} - (I + \gamma_{i-1/2}(x_i - x_{i-1/2})A_{i-1/2}) \mathbf{J}_{i-1/2} = qb_i \mathbf{R}_i$$

The function  $\gamma$  in (4.2) depends on the eigenvalue  $\lambda$ , and therefore we write  $\gamma = \gamma_{i+1/2}$  for the matrix  $A = A_{i+1/2}$ ; and likewise for  $\gamma_{i-1/2}$ . In the following however, we will omit the subscripts  $i \pm 1/2$  for convenience.

Consider the current relations (3.10). Substitution of equation (4.1) for the matrix exponent gives

(4.3a) 
$$\mathbf{J}_{i+1/2} = (I + G_{i+1/2}A_{i+1/2})^{-1} \mathbf{\tilde{J}}_{i+1/2},$$
  
(4.3b)  $\mathbf{\tilde{J}}_{i+1/2} = E_{i+1/2}^{-1} (\mathbf{\tilde{u}}_{i+1} - \mathbf{\tilde{u}}_i).$ 

In (4.3b),  $\tilde{\mathbf{J}}_{i+1/2}$  is the current density in the case that avalanche generation is neglected. The 2 × 2 diagonal matrices E, F and G, occurring in the computation of  $\mathbf{J}_{i+1/2}$ , are defined by

(4.4a) 
$$E_{i+1/2} = \int_{x_i}^{x_{i+1}} D^{-1} dx,$$
  
(4.4b)  $F_{i+1/2} = \int_{x_i}^{x_{i+1}} \gamma(x - x_{i+1/2}) D^{-1} dx,$   
(4.4c)  $G_{i+1/2} = E_{i+1/2}^{-1} F_{i+1/2}.$ 

The final discretisation scheme, after substitution of (4.3a) in (4.2), reads

(4.5) 
$$(I + \gamma(x_i - x_{i+1/2})A_{i+1/2}) (I + G_{i+1/2}A_{i+1/2})^{-1} \tilde{\mathbf{J}}_{i+1/2} - (I + \gamma(x_i - x_{i-1/2})A_{i-1/2}) (I + G_{i-1/2}A_{i-1/2})^{-1} \tilde{\mathbf{J}}_{i-1/2} = qb_i \mathbf{R}_i$$

Thus, to complete the scheme, we still have to compute the current densities  $\tilde{J}_{i+1/2}$  and the matrix G.

Computation of  $\mathbf{J}_{i+1/2}$  gives the standard Scharfetter-Gummel expressions for the current densities. In the non-isothermal case they read ([12])

$$\begin{array}{ll} (4.6a) \quad \tilde{J}_{n,i+1/2} = \frac{q D_{n,i+1/2}}{h_{i+1}} \bar{T}(x_i, x_{i+1}) \left( B(\delta_n) \frac{n_{i+1}}{T_{i+1}} - B(-\delta_n) \frac{n_i}{T_i} \right), \\ \\ \delta_n = \left( (\psi_{i+1} - \psi_i) - (r+2) (U_{T,i+1} - U_{T,i}) \right) / \bar{U}_T(x_i, x_{i+1}), \\ (4.6b) \quad \tilde{J}_{p,i+1/2} = -\frac{q D_{p,i+1/2}}{h_{i+1}} \bar{T}(x_i, x_{i+1}) \left( B(-\delta_p) \frac{p_{i+1}}{T_{i+1}} - B(\delta_p) \frac{p_i}{T_i} \right), \end{array}$$

$$\delta_p = \left( (\psi_{i+1} - \psi_i) + (r+2)(U_{T,i+1} - U_{T,i}) \right) / \bar{U}_T(x_i, x_{i+1}).$$

B(z) is the Bernoulli function defined by  $B(z) = z/(e^z - 1)$ . In the derivation of (4.6) we have assumed that on the interval  $[x_i, x_{i+1}]$ , the potential  $\psi$  and the temperature T are linear and that the diffusion coefficients  $D_n$  and  $D_p$  are constant. The equations (4.6) might lead to cancellation problems; see e.g. [4], where this problem is discussed for the isothermal case. An alternative formulation for the current densities, expressed in the variables  $\tilde{\varphi}_n$  and  $\tilde{\varphi}_p$  is

$$\begin{array}{ll} (4.7a) \quad \tilde{J}_{n,i+1/2} = \frac{q D_{n,i+1/2}}{h_{i+1}} \bar{T}(x_i, x_{i+1}) B(-\delta_n) \delta(\tilde{\varphi}_{n,i} - \tilde{\varphi}_{n,i+1}) \frac{n_i}{T_i}, \\ (4.7b) \quad \tilde{J}_{p,i+1/2} = -\frac{q D_{p,i+1/2}}{h_{i+1}} \tilde{T}(x_i, x_{i+1}) B(\delta_p) \delta(\tilde{\varphi}_{p,i+1} - \tilde{\varphi}_{p,i}) \frac{p_i}{T_i}, \end{array}$$

where the function  $\delta(z)$  is defined by  $\delta(z) = e^z - 1$ . In order to avoid cancellation problems,  $\delta(z)$  should be developed in a Taylor series for small values of z. Similar expressions for  $\tilde{J}_{n,i+1/2}$  with  $\frac{n_i}{T_i}$  replaced by  $\frac{n_{i+1}}{T_{i+1}}$  or  $\left(\frac{n_i n_{i+1}}{T_i T_{i+1}}\right)^{1/2}$  can be easily derived. The same holds, mutatis mutandis, for  $\tilde{J}_{p,i+1/2}$ .

Finally, consider the computation of the diagonal matrix G. A simple calculation shows (cf. (4.4)) that the matrix elements  $G_{11}$  and  $G_{22}$  are given by

(4.8a) 
$$G_{11,i+1/2} = \frac{\int_{x_i}^{x_{i+1}} \gamma(x - x_{i+1/2}) e^{-a_n} dx}{\int_{x_i}^{x_{i+1}} e^{-a_n} dx},$$
  
(4.8b)  $G_{22,i+1/2} = \frac{\int_{x_i}^{x_{i+1}} \gamma(x - x_{i+1/2}) e^{a_p} dx}{\int_{x_i}^{x_{i+1}} e^{a_p} dx}.$ 

In the isothermal case, the computation of  $G_{11}$  and  $G_{22}$  is straightforward, and we find, with  $\Delta = (\psi_{i+1} - \psi_i)/(2U_T)$ ,

(4.9a) 
$$G_{11,i+1/2} = -(x_{i+1/2} - x_i)g(\Delta, -\lambda(x_{i+1/2} - x_i))),$$
  
(4.9b)  $G_{22,i+1/2} = (x_{i+1/2} - x_i)g(\Delta, \lambda(x_{i+1/2} - x_i))),$ 

where  $\lambda$  is a short notation for  $\lambda_{i+1/2}$ . The function g(x, y) in (4.9) is defined by

(4.10a) 
$$g(x,y) = \frac{f(x+y) - f(x)}{yf(x)},$$

with

(4.10b) 
$$f(z) = \frac{\sinh(z)}{z}.$$

In the computation of g(x, y), expression (4.10a) has to be replaced by a Taylor series for small values of y. Also f(z) has to be developed in a Taylor series for small values of z. However, in the non-isothermal case, the integrals in the denominators of (4.8) can not be evaluated exactly if we assume that T(x) (or  $U_T(x)$ ) is a linear function on  $[x_i, x_{i+1}]$ . Therefore, only in the computation of  $G_{11}$  and  $G_{22}$ , we replace  $U_T$  by a suitably chosen average  $\overline{U}_T$ , e.g.  $\overline{U}_T = \frac{1}{2}(U_{T,i} + U_{T,i+1})$ . Herewith we tacitly assume that T is a mildly varying function. This is correct if we ignore hot electron effects. Computation of  $G_{11}$  and  $G_{22}$  then gives

$$(4.11a) \quad G_{11,i+1/2} = -(x_{i+1/2} - x_i)g(\Delta_n, -\lambda(x_{i+1/2} - x_i)),$$
  

$$\Delta_n = (\psi_{n,i+1} - \psi_{n,i})/(2\bar{U}_T),$$
  

$$(4.11b) \quad G_{22,i+1/2} = (x_{i+1/2} - x_i)g(\Delta_p, \lambda(x_{i+1/2} - x_i)),$$
  

$$\Delta_p = (\psi_{p,i+1} - \psi_{p,i})/(2\bar{U}_T).$$

# 5 Extension of the exponential fitting scheme to a 2-dimensional rectangular mesh

In Section 3 we have derived an exponential fitting scheme for the 1-dimensional semiconductor device equations, modeling avalanche generation and a variable device temperature. Now we discuss the extension of this scheme to a 2-dimensional rectangular mesh. For a triangular mesh, the derivation of the scheme is more complicated.

First we discuss the isothermal case. Consider the continuity equations (2.2) and the current relations (2.17). The current densities  $\mathbf{J}_n = (J_{nx}, J_{ny})^T$  and  $\mathbf{J}_p = (J_{px}, J_{py})^T$  are now proper vectors, and their directions are determined by  $\nabla \varphi_n$  and  $\nabla \varphi_p$ , respectively. Let  $\mathbf{s}_n = (\mathbf{s}_{nx}, \mathbf{s}_{ny})^T$  and  $\mathbf{s}_p = (s_{px}, s_{py})^T$  be the unit vectors in the direction of respectively  $\mathbf{J}_n$  and  $\mathbf{J}_p$ , then obviously

(5.1) 
$$\mathbf{s}_n = -\frac{\nabla \varphi_n}{|\nabla \varphi_n|}, \mathbf{s}_p = -\frac{\nabla \varphi_p}{|\nabla \varphi_p|}.$$

The absolute values of the current densities are then given by the inner products  $|\mathbf{J}_n| = (\mathbf{s}_n, \mathbf{J}_n)$  and  $|\mathbf{J}_p| = (\mathbf{s}_p, \mathbf{J}_p)$ , and thus the continuity equations read

(5.2a) 
$$\nabla \cdot \mathbf{J}_n = -\alpha_n(\mathbf{s}_n, \mathbf{J}_n) - \alpha_p(\mathbf{s}_p, \mathbf{J}_p) + qR,$$
  
(5.2b)  $\nabla \cdot \mathbf{J}_p = \alpha_n(\mathbf{s}_n, \mathbf{J}_n) + \alpha_p(\mathbf{s}_p, \mathbf{J}_p) - qR.$ 

Define the vectors  $\mathbf{J}_x = (J_{nx}, J_{px})^T$  and  $\mathbf{J}_y = (J_{ny}, J_{py})^T$ , and the 2 × 2 matrix  $J = (\mathbf{J}_n, \mathbf{J}_p)$ . Rearranging terms, equation (5.2) can be written in the following two equivalent forms

(5.3a) 
$$\nabla \cdot J = A_x \mathbf{J}_x + A_y \mathbf{J}_y + q \mathbf{R},$$

or

(

(5.3b) 
$$\left(\frac{\partial \mathbf{J}_x}{\partial x} - A_x \mathbf{J}_x\right) + \left(\frac{\partial \mathbf{J}_y}{\partial y} - A_y \mathbf{J}_y\right) = q\mathbf{R},$$

where the matrices  $A_x$  and  $A_y$  are defined by

(5.3c) 
$$A_x = \begin{pmatrix} -\alpha_n s_{nx} & -\alpha_p s_{px} \\ \alpha_n s_{nx} & \alpha_p s_{px} \end{pmatrix}, A_y = \begin{pmatrix} -\alpha_n s_{ny} & -\alpha_p s_{py} \\ \alpha_n s_{ny} & \alpha_p s_{py} \end{pmatrix}.$$

In (5.3a),  $\nabla \cdot J$  is defined by  $\nabla \cdot J = (\nabla \cdot \mathbf{J}_n, \nabla \cdot \mathbf{J}_p)^T$ . This form of the continuity equations can be used to generalise the exponential fitting scheme on a 2-dimensional rectangular mesh.

We apply the box method to equation (5.3a). Consider the box  $B_{ij} = [x_{i-1/2}, x_{i+1/2}] \times [y_{j-1/2}, y_{j+1/2}]$  around mesh point  $(x_i, y_j)$ ; see Figure 2. Integration of (5.3a) over box  $B_{ij}$  gives

(5.4) 
$$\int \int_{B_{ij}} \nabla \cdot J dS = \int \int_{B_{ij}} (A_x \mathbf{J}_x + A_y \mathbf{J}_y) dS + q \int \int_{B_{ij}} \mathbf{R} dS.$$

Using Gauss' law, the first integral in (5.4) can be reduced to a contour integral:

(5.5) 
$$\int \int_{B_{ij}} \nabla \cdot J dS = \oint_{\partial B_{ij}} (\nu_x \mathbf{J}_x + \nu_y \mathbf{J}_y) ds,$$

where  $\nu = (\nu_x, \nu_y)^T$  is the unit outward normal to the boundary  $\partial B_{ij}$ . The contour integral in (5.5) and the third integral in (5.4) are approximated by the lowest order quadrature rules. Thus, the approximation of the contour integral is

(5.6) 
$$\oint_{\partial B_{ij}} (\nu_x \mathbf{J}_x + \nu_y \mathbf{J}_y) ds = (y_{j+1/2} - y_{j-1/2}) (\mathbf{J}_{x,i+1/2,j} - \mathbf{J}_{x,i-1/2,j}) + (x_{i+1/2} - x_{i-1/2}) (\mathbf{J}_{y,i,j+1/2} - \mathbf{J}_{y,i,j-1/2}).$$

In (5.6),  $\mathbf{J}_{x,i+1/2,j} = \mathbf{J}_x(x_{i+1/2}, y_j)$ , etc. The integral of the recombination rate **R**, the third integral in (5.4), is approximated by  $b_{ij}\mathbf{R}_{ij}$ , where  $b_{ij} = (x_{i+1/2} - x_{i-1/2})(y_{j+1/2} - y_{j-1/2})$  is the area of box  $B_{ij}$  and  $\mathbf{R}_{ij} = \mathbf{R}(x_i, y_j)$ .

In order to compute the second integral in (5.4), we have to know the variation of  $J_x$  and  $J_y$  over  $B_{ij}$ . By analogy with the 1-dimensional case, we assume that for  $(x, y) \in B_{ij}$ ,  $J_x$  and  $J_y$  satisfy the following equations

(5.7a) 
$$\frac{\partial \mathbf{J}_x}{\partial x} - A_x \mathbf{J}_x = \mathbf{0}, \frac{\partial \mathbf{J}_x}{\partial y} = \mathbf{0},$$
  
(5.7b)  $\frac{\partial \mathbf{J}_y}{\partial x} = \mathbf{0}, \frac{\partial \mathbf{J}_y}{\partial y} - A_y \mathbf{J}_y = \mathbf{0}.$ 

This means that  $\mathbf{J}_x$  is an exponentially varying function in the x-direction and is constant in the y-direction. Likewise,  $\mathbf{J}_y$  is constant in x-direction and exponentially varying in y-direction. Thus, referring to equation (5.3b), both the x-term and the yterm in the homogenous continuity equation are separately set equal to zero. Assuming piecewise constant matrices  $A_x$  and  $A_y$ , the equations (5.7) can be solved easily and subsequently, the second integral in (5.4) can be computed. Since  $A_x$  depends on the x-derivatives of  $\psi$ ,  $\varphi_n$  and  $\varphi_p$ , a suitable choice is to take  $A_x$  constant on the rectangle  $[x_i, x_{i+1}] \times [y_{j-1/2}, y_{j+1/2}]$  (see Figure 2); we write  $A_x = A_{x,i+1/2,j}$ . Likewise, we take  $A_y = A_{y,i,j+1/2}$  constant on the rectangle  $[x_{i-1/2}, x_{i+1/2}] \times [y_j, y_{j+1}]$ . Thus, the integral of  $A_x \mathbf{J}_x + A_y \mathbf{J}_y$  over  $B_{ij}$  can be split into four parts in a natural way. As an example, we present the integral of  $A_x \mathbf{J}_x$  over the right half  $B_{ij}^r$  of the box  $B_{ij}$ 

(5.8) 
$$\int \int_{B_{ij}^r} A_x \mathbf{J}_x dS = (y_{j+1/2} - y_{j-1/2}) \left( I - e^{(x_i - x_{i+1/2})A_{x,i+1/2,j}} \right) \mathbf{J}_{x,i+1/2,j}.$$

From the foregoing, we get the following discrete continuity equations

$$(5.9) \quad (y_{j+1/2} - y_{j-1/2}) \left( e^{(x_i - x_{i+1/2})A_{x,i+1/2,j}} \mathbf{J}_{x,i+1/2,j} - e^{(x_i - x_{i-1/2})A_{x,i-1/2,j}} \mathbf{J}_{x,i-1/2,j} \right) + (x_{i+1/2} - x_{i-1/2}) \left( e^{(y_j - y_{j+1/2})A_{y,i,j+1/2}} \mathbf{J}_{y,i,j+1/2} - e^{(y_j - y_{j-1/2})A_{y,i,j-1/2}} \mathbf{J}_{y,i,j-1/2} \right) = q b_{ij} \mathbf{R}_{ij}.$$

This equation is the 2-dimensional analogue of equation (3.8).

The computation of the current densities is divided into the separate computation of the x-components  $J_x$  and the y-components  $J_y$ . Consider the computation of  $J_x$ . From the current relations (2.18), it is easy to see that  $J_x$  satisfies

$$(5.10) \quad \mathbf{J}_x = D \frac{\partial \mathbf{u}}{\partial x},$$

where the matrix D is defined in (3.9b). Let  $x \in [x_i, x_{i+1}]$  and  $y = y_j$ , and assume that  $J_x$  satisfies (5.7a). Then, analogous to the 1-dimensional case,  $J_{x,i+1/2,j}$  can be computed from (5.10), and we find

(5.11) 
$$\mathbf{J}_{x,i+1/2,j} = \left(\int_{x_i}^{x_{i+1}} D^{-1} e^{(x_i - x_{i+1/2})A_{x,i+1/2,j}} dx\right)^{-1} (\mathbf{u}_{i+1,j} - \mathbf{u}_{ij}).$$

A similar expression can be obtained for  $J_y$ .

Now, consider the non-isothermal case. In the following, we use the notation  $\partial_x = \frac{\partial}{\partial x}$  and  $\partial_y = \frac{\partial}{\partial y}$ . The major difference between the discretisation schemes for the isothermal and the non-isothermal case is the computation of the unit vectors  $\mathbf{s}_n$  and  $\mathbf{s}_p$ . In analogy with the 1-dimensional case, cf. (3.12), we try the following representation for the current densities:

(5.12a) 
$$\mathbf{J}_n = q D_n e^{a_n} \nabla (n e^{-a_n}),$$
  
(5.12b)  $\mathbf{J}_p = -q D_p e^{-a_n} \nabla (p e^{a_p}).$ 

However, since  $\partial_y(\partial_x a_n) = \partial_x(\partial_y a_n)$  and  $\partial_y(\partial_x a_p) = \partial_x(\partial_y a_p)$ , equation (5.12) gives rise to the following necessary condition

(5.13) 
$$\begin{vmatrix} \partial_x \psi & \partial_x T \\ \partial_y \psi & \partial_y T \end{vmatrix} = 0,$$

and in general, this condition only holds for constant T. Therefore, instead of (5.12), we have to assume the representations

(5.14a) 
$$J_{nx} = qD_n e^{a_{nx}} \partial_x (ne^{-a_{nx}}), J_{ny} = qD_n e^{a_{ny}} \partial_y (ne^{-a_{ny}}),$$
  
(5.14b) 
$$J_{px} = -qD_p e^{-a_{px}} \partial_x (pe^{a_{px}}), J_{py} = -qD_p e^{-a_{py}} \partial_y (pe^{a_{py}}).$$

The computation of the variables  $a_{nx}$ , etc. is straightforward and completely analogous to the 1-dimensional case. Let the variables  $\varphi_{nx}, \varphi_{ny}, \varphi_{px}$  and  $\varphi_{py}$  be defined by, cf. (3.14),

(5.15a) 
$$\varphi_{nx} = a_{nx} - \ln\left(\frac{n}{n_{int}}\right), \varphi_{ny} = a_{ny} - \ln\left(\frac{n}{n_{int}}\right),$$
  
(5.15b)  $\varphi_{px} = a_{px} + \ln\left(\frac{p}{n_{int}}\right), \varphi_{py} = a_{py} + \ln\left(\frac{p}{n_{int}}\right).$ 

Then we obtain the following expressions for the current densities

(5.16a) 
$$\mathbf{J}_{n} = -qD_{n}n \left( \begin{array}{c} \partial_{x}\varphi_{nx} \\ \partial_{y}\varphi_{ny} \end{array} \right),$$
  
(5.16b)  $\mathbf{J}_{p} = -qD_{p}p \left( \begin{array}{c} \partial_{x}\varphi_{px} \\ \partial_{y}\varphi_{py} \end{array} \right).$ 

The unit vectors  $s_n$  and  $s_p$  can be readily determined from (5.16). Further, the discretisation of the continuity equations proceeds in exactly the same way as in the isothermal case.

Concerning the computation of the current densities, we note the following. Let the variables  $u_x, u_y, v_x$  and  $v_y$  be defined by, cf. (3.15),

- (5.17a)  $u_x = e^{-\varphi_{nx}}, u_y = e^{-\varphi_{ny}},$
- (5.17b)  $v_x = e^{\varphi_{px}}, v_y = e^{\varphi_{py}},$

then the current relations can be written as

(5.18a) 
$$\mathbf{J}_x = D_x \partial_x \mathbf{u}_x, \mathbf{J}_y = D_y \partial_y \mathbf{u}_y,$$

where  $\mathbf{u}_x = (u_x, v_x)^T$  and  $\mathbf{u}_y = (u_y, v_y)^T$ , and where the matrices  $D_x$  and  $D_y$  are defined by

(5.18b) 
$$D_x = q n_{int} \begin{pmatrix} D_n e^{a_{nx}} & 0 \\ 0 & -D_p e^{-a_{px}} \end{pmatrix}, D_y = q n_{int} \begin{pmatrix} D_n e^{a_{ny}} & 0 \\ 0 & -D_p e^{-a_{py}} \end{pmatrix}$$

The computation of the current densities is now completely analogous to the isothermal case.

# 6 Conclusions

In this paper we have presented a numerical scheme for the electrothermal device equations, specifically for the simulation of avalanche generation, in which case the current densities are exponentially varying functions of the spatial variables. Therefore, we have extended the box scheme and the standard Scharfetter-Gummel scheme, using the assumption that the current densities are exponentially varying functions in each mesh interval. On the other hand, in the standard Scharfetter-Gummel scheme the current densities are assumed to be piecewise constant. As a consequence, the scheme will give much better predictions for the currents in a device than the standard scheme, when avalanche generation is the predominant generation mechanism. This is confirmed in [18], where the scheme is applied to the isothermal device equations. Finally, it should be noted that the current densities can be easily computed from the standard Scharfetter-Gummel expressions.

#### Appendix: Nomenclature

- $\psi$ electrostatic potential (V)
- electron concentration  $(cm^{-3})$ n
- hole concentration  $(cm^{-3})$ p
- Tdevice temperature (K)
- quasi-Fermi potential for electrons (V) $\varphi_n$
- quasi-Fermi potential for holes (V) $\varphi_p$
- Slotboom variables u, v
- Е electric field (V/cm)
- $\mathbf{J}_n$ electron current density  $(A/cm^2)$
- $\mathbf{J}_p$ hole current density  $(A/cm^2)$
- space charge density  $(C/cm^3)$ ρ
- D doping profile  $(cm^{-3})$
- Ν total impurity concentration  $(cm^{-3})$
- $N_D$ ionised donor concentration  $(cm^{-3})$
- ionised acceptor concentration  $(cm^{-3})$  $N_A$
- ionisation rate for electrons  $(cm^{-1})$  $\alpha_n$
- ionisation rate for holes  $(cm^{-1})$  $\alpha_p$
- recombination/generation rate (excluding avalanche generation)  $(cm^{-3}s^{-1})$ R
- thermal conductivity (W/cmK)κ
- Η heat generation rate  $(W/cm^3)$
- electron mobility  $(cm^2/Vs)$  $\mu_n$
- hole mobility  $(cm^2/Vs)$  $\mu_p$
- $D_n$ diffusion coefficient for electrons  $(cm^2/s)$
- diffusion coefficient for holes  $(cm^2/s)$
- thermal diffusion coefficient for electrons  $(cm^2/Ks)$
- $D_p$  $D_n^T$  $D_p^T$ thermal diffusion coefficient for holes  $(cm^2/Ks)$
- ε permittivity (C/Vcm)
- elementary charge (C)q k
- Boltzmann constant (VC/K)



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Figure 1: The box corresponding to  $x_i$ .



Figure 2: The box corresponding to  $x_{ij}$ .

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