

# Amorphous Silicon Device Simulation by an Adapted Gummel Method

M. KEMP, C. G. TANNOUS, AND M. MEUNIER, MEMBER, IEEE

**Abstract**—The operation of hydrogenated amorphous silicon devices depends crucially on the interplay between the dynamics of free and trapped carriers. This is due to a density of acceptor and donor states present in the mobility gap of amorphous materials. We show that Gummel's method used for the simulation of crystalline-material-based devices has to be modified in order to account for this interplay. We identify the midgap density of states as the parameter controlling the nature of the dynamics of the carriers and illustrate this with two examples: the 1D Schottky diode and the 2D static induction transistor.

GUMMEL'S method is based on a highly effective decoupling algorithm that is heavily used in crystalline semiconductor device simulation. Using a nonlinear modification of Poisson's equation by taking into account the exponential dependence of electron and hole density on electrostatic potential, Gummel [1] proposed an iterative scheme that was recently proven [2] rigorously to be convergent for realistic device geometries in one, two, and three dimensions. In hydrogenated amorphous silicon (a-Si:H) based devices the dynamics of trapped electrons and holes are coupled to the dynamics of conduction electrons and holes and one must adapt the classical Gummel method to account for this fact. In this paper we derive this adaptation, show that the midgap density of states primarily controls the nature of carrier dynamics, and illustrate our viewpoint with two a-Si:H based devices: a 1D Schottky diode and a 2D static induction transistor (SIT).

Numerical simulation of semiconductor devices consists of solving the following set of three coupled partial differential equations:

$$\nabla^2 \psi = -\frac{q}{\epsilon} (p - n + p_i - n_i + C) \quad (1)$$

$$q \frac{\partial n}{\partial t} = \text{div } \vec{J}_n - qR_n \quad (2)$$

$$q \frac{\partial p}{\partial t} = -\text{div } \vec{J}_p - qR_p \quad (3)$$

with appropriate boundary and initial conditions, where  $\psi$  is the electrostatic potential,  $n$  the electron density,  $p$  the

hole density,  $n_i$  the trapped electron density,  $p_i$  the trapped hole density,  $C$  the doping profile,  $\vec{J}_n$  and  $\vec{J}_p$  the electron and hole current density,  $R_n$  and  $R_p$  the net recombination rate of conduction electrons and holes,  $q$  the electronic charge, and  $\epsilon$  the dielectric permittivity. In order to ease the comparison, let us first review the standard nonadapted Gummel method.

Consider a trap-free crystalline semiconductor for which Poisson's equation reads

$$\nabla^2 \psi = -\frac{q}{\epsilon} (p - n + C). \quad (4)$$

The numerical solution to the set of equations (2), (3), and (4) could be obtained by replacing the field equations by a finite difference set of algebraic equations, guessing initial values of  $\psi$ ,  $n$ ,  $p$  at the grid nodes and then successively solving the set of equations using the best available values of  $\psi$ ,  $n$ ,  $p$  until convergence. This scheme may prove successful; its convergence rate, however, may turn out to be extremely low. Gummel [1] devised a way to increase the speed of convergence by taking advantage of the equilibrium dependence of  $n$  and  $p$  on the electrostatic potential. Using the following change of variables:

$$\begin{aligned} n &= u \exp\left(\frac{q\psi}{k_B T}\right) \\ p &= v \exp\left(-\frac{q\psi}{k_B T}\right) \end{aligned} \quad (5)$$

and substituting in (4), one obtains

$$\nabla^2 \psi = -\frac{q}{\epsilon} \left( v \exp\left(-\frac{q\psi}{k_B T}\right) - u \exp\left(\frac{q\psi}{k_B T}\right) + C \right) \quad (6)$$

where  $k_B$  and  $T$  denote Boltzmann's constant and temperature, respectively.

Let  $\psi^K$ ,  $n^K$ , and  $p^K$  be the values obtained at the  $K$ th iterative step. Gummel used the hypothesis that  $u^{K+1}$  and  $v^{K+1}$  are identical to  $u^K$  and  $v^K$  in order to decouple the equations. Defining  $\Delta^{K+1} \psi = \psi^{K+1} - \psi^K$  and rewriting (6) in terms of  $\psi^{K+1}$ ,  $n^K$ ,  $p^K$ , he obtained

$$\nabla^2 \psi^{K+1} = -\frac{q}{\epsilon} (\bar{p}_K - \bar{n}_K + C) \quad (7)$$

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The authors are with the Groupe des Couches Minces and the Department of Engineering Physics, Ecole Polytechnique de Montréal, Montréal, Canada H3C 3A7.

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where

$$\begin{aligned} \bar{n}_K &= n^K \exp\left(\frac{q}{k_B T} \Delta^{K+1} \psi\right) \\ \bar{p}_K &= p^K \exp\left(-\frac{q}{k_B T} \Delta^{K+1} \psi\right) \end{aligned} \quad (8)$$

which is the form of Poisson's equation used in Gummel's iterative procedure. The original Gummel's algorithm is obtained in replacing the exponentials by their first-order Taylor expansion yielding

$$\begin{aligned} \nabla^2 \psi^{K+1} &= -\frac{q}{\epsilon} \left[ p^K \left( 1 - \frac{q}{k_B T} \Delta^{K+1} \psi \right) \right. \\ &\quad \left. - n^K \left( 1 + \frac{q}{k_B T} \Delta^{K+1} \psi \right) + C \right]. \end{aligned} \quad (9)$$

Consider now an a-Si:H based device. In addition to the doping term  $C$  in (4) there appear two new terms: the trapped electron and hole charge densities. It is imperative to consider now the dynamics of the trapped carriers. The amorphous material is characterized by a density of acceptor and donor localized states in the mobility gap. The filling of these states is governed by a statistical occupation function that in general is a functional of the free-carrier densities. For example, Simmons and Taylor [3] generalizing the Shockley-Read-Hall (SRH) treatment obtained in the steady state the following occupation function:

$$f_i(\epsilon, n, p) = \frac{\bar{n} + e_p}{\bar{n} + \bar{p} + e_n + e_p} \quad (10)$$

where  $\bar{n} \equiv v_{th} \sigma_n n$ ,  $\bar{p} \equiv v_{th} \sigma_p p$ ,  $v_{th}$  is the thermal velocity,  $\sigma_n$  and  $\sigma_p$  the cross section of capture of electrons and holes,  $e_n$  and  $e_p$  the emission rates for trapped electrons and holes, and where  $\sigma_n$ ,  $\sigma_p$ ,  $e_n$ , and  $e_p$  are functions of the energy of the trap level. The density of trapped electrons and holes is obtained [4] by integrating over the gap this function times the density of states

$$n_i(n, p) = \sum_j \int_{\epsilon_v}^{\epsilon_c} d\epsilon g_{aj}(\epsilon) f_i^{(j)}(\epsilon, n, p) \quad (11a)$$

$$p_i(n, p) = \sum_j \int_{\epsilon_v}^{\epsilon_c} d\epsilon g_{dj}(\epsilon) (1 - f_i^{(j)}(\epsilon, n, p)) \quad (11b)$$

where summation extends over acceptor species for  $n_i$  and over donor species for  $p_i$  with their corresponding density of states  $g_{aj}$  and  $g_{dj}$ , respectively, and occupation function  $f_i^{(j)}$  where  $j$  denotes the  $j$ th species. It is thus seen that the trapped carrier densities are functionals of the free-carrier densities. In the spirit of Gummel's derivation one has to take account of this dependence in order to correctly derive the Poisson equation suitable for the simulation of a-Si:H based devices.

Using (5), the space-charge density is rewritten

$$\rho = v \exp\left(-\frac{q\psi}{k_B T}\right) - u \exp\left(\frac{q\psi}{k_B T}\right) + \rho_i + C \quad (12)$$

where  $\rho_i = p_i - n_i$  is a function of  $u \exp(q\psi/k_B T)$  and  $v \exp(-q\psi/k_B T)$ . With a procedure identical to the one used to obtain (7), one gets

$$\nabla^2 \psi^{K+1} = -\frac{q}{\epsilon} [\bar{p}_K - \bar{n}_K + \rho_i(\bar{n}_K, \bar{p}_K) + C]. \quad (13)$$

Our numerical experiments performed on the basis of the algorithm given in (13) tend to show that the region of attraction of the discretized form of this nonlinear equation is extremely small. Instead of solving the nonlinear set of equations, we linearize it for use in the iterative scheme. To first order, one gets

$$\begin{aligned} \nabla^2 \psi^{K+1} &= -\frac{q}{\epsilon} \left[ p^K \left( 1 - \frac{q}{k_B T} \Delta^{K+1} \psi \right) \right. \\ &\quad \left. - n^K \left( 1 + \frac{q}{k_B T} \Delta^{K+1} \psi \right) + \rho_i(n^K, p^K) \right. \\ &\quad \left. + C + \frac{q}{k_B T} \Delta^{K+1} \psi \left[ n^K \frac{\partial}{\partial n} \rho_i(n^K, p^K) \right. \right. \\ &\quad \left. \left. - p^K \frac{\partial}{\partial p} \rho_i(n^K, p^K) \right] \right]. \end{aligned} \quad (14)$$

Note that the first four terms of the RHS are identical to the three terms of (9) if one includes  $\rho_i$  in the doping function  $C$  of the crystalline case. The remaining terms are new and are a consequence of the presence of a density of localized states. Their effect on the convergence of the numerical scheme appears to be very important as can be seen in the following. Using SRH statistics, one gets

$$\begin{aligned} \frac{\partial}{\partial n} \rho_i &= -\sum_j v_{th} \sigma_{nj} \int_{\epsilon_v}^{\epsilon_c} d\epsilon g_{aj}(\epsilon) \frac{1 - f_i^{(j)}(\epsilon, n, p)}{(\bar{n} + \bar{p} + e_n + e_p)_j} \\ &\quad - \sum_j v_{th} \sigma_{pj} \int_{\epsilon_v}^{\epsilon_c} d\epsilon g_{dj}(\epsilon) \frac{1 - f_i^{(j)}(\epsilon, n, p)}{(\bar{n} + \bar{p} + e_n + e_p)_j} \end{aligned} \quad (15a)$$

$$\begin{aligned} \frac{\partial}{\partial p} \rho_i &= \sum_j v_{th} \sigma_{pj} \int_{\epsilon_v}^{\epsilon_c} d\epsilon g_{dj}(\epsilon) \frac{f_i^{(j)}(\epsilon, n, p)}{(\bar{n} + \bar{p} + e_n + e_p)_j} \\ &\quad + \sum_j v_{th} \sigma_{nj} \int_{\epsilon_v}^{\epsilon_c} d\epsilon g_{aj}(\epsilon) \frac{f_i^{(j)}(\epsilon, n, p)}{(\bar{n} + \bar{p} + e_n + e_p)_j} \end{aligned} \quad (15b)$$

where in both equations the first summation extends over donor species and the second one extends over acceptor species. The emission rates are given by

$$e_n(\epsilon) = n_i v_{th} \sigma_n \exp\left(\frac{\epsilon - \epsilon_i}{k_B T}\right) \quad (16a)$$

$$e_p(\epsilon) = n_i v_{th} \sigma_p \exp\left(\frac{\epsilon_i - \epsilon}{k_B T}\right) \quad (16b)$$

where  $n_i$  is the intrinsic concentration and  $\epsilon_i$  the intrinsic level. As an example of the orders of magnitude involved,



a simple calculation for a-Si:H yields the following: the major contribution to the integrals (15a) and (15b) comes from levels near midgap due to the exponential dependence of the emission rates on energy. If one approximates the integrands by their values at midgap over a domain of extent  $5 k_B T$  around midgap, and if one takes equilibrium values for  $n$  and  $p$  as in the intrinsic case, that is  $n = 3 \times 10^9 \text{ cm}^{-3}$ ,  $p = 9 \times 10^5 \text{ cm}^{-3}$ ; further, if one takes  $\sigma_n = \sigma_p$  and  $f_i(\epsilon_i) = 1/2$ , one finally obtains

$$\frac{\partial}{\partial n} \rho_i = \frac{\partial}{\partial p} \rho_i \equiv 1 \times 10^{-11} g(\epsilon_i) \quad (17)$$

where the density of states is expressed in reciprocal cubic centimeters per electronvolt.

Rearranging (14) and defining  $\Delta p = 1 + \partial \rho_i / \partial p$  and  $\Delta n = 1 - \partial \rho_i / \partial n$ . Then

$$\nabla^2 \psi^{K+1} = -\frac{q}{\epsilon} \left[ p^K - n^K + \rho_i(n^K, p^K) + C - \frac{q}{k_B T} \Delta^{K+1} \psi (p^K \Delta p + n^K \Delta n) \right]. \quad (18)$$

If one neglects the dependence of  $\rho_i$  on  $n$  and  $p$  as in the case of the standard Gummel method, then  $\Delta p$  and  $\Delta n$  are strictly equal to 1. In the case of a-Si:H with a typical midgap density of states of  $10^{16} \text{ cm}^{-3}/\text{eV}$ ,  $\Delta p$  and  $\Delta n$  are very large and the solution to the iteration problem (18) is completely dominated by this contribution. Hence, the convergence of the numerical scheme is extremely sensitive to the value of the midgap density of states.

We illustrate our point of view in two cases: the a-Si:H based 1D Schottky diode and the a-Si:H based 2D SIT, in the steady state [5]. We use a density of states consisting of exponential band tail species with Gaussian deep-level species. Occupation of these levels and recombination rates are governed by SRH statistics. The simulation is done for the Schottky diode with 0 V on the Schottky contact and -2 V on the ohmic one and for the SIT with 0 V on source and drain and -1 V on the gate.

In Fig. 1(a) and (b) the maximum relative correction of the electrostatic potential defined as

$$C_{\max}^K = \max \left| \frac{\psi_{ij}^K - \psi_{ij}^{K-1}}{\psi_{ij}^K} \right| \quad (19)$$

is displayed as a function of the iteration step  $K$  using both adapted and nonadapted schemes for the two types of devices studied. When the defect concentration near midgap is low, we checked that both numerical schemes indeed converge at the same speed. When the density of states at midgap increases (above  $5 \times 10^{16} \text{ cm}^{-3}/\text{eV}$ ) we observed a major change in the rate of convergence of the two methods. While the nonadapted method started slowing down or even inducing an oscillatory behavior of  $C_{\max}^K$  versus  $K$ , the adapted method kept having a relatively high rate of convergence.

To conclude, we have presented and derived the adaptation of Gummel's method for the simulation of a-Si:H

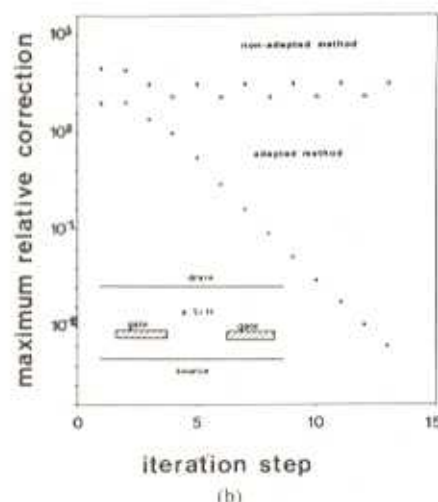
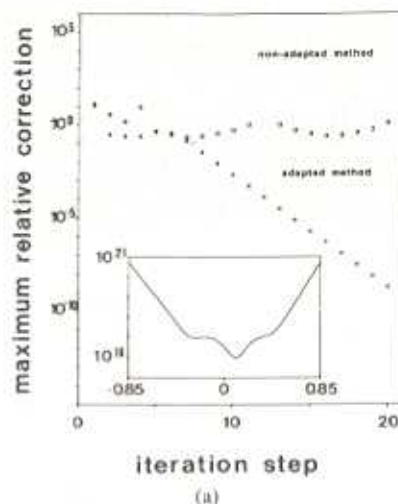


Fig. 1. Evolution of the maximum relative correction of the electrostatic potential as a function of iteration step for adapted and nonadapted Gummel method for: (a) 1D Schottky diode  $3 \mu\text{m}$  long and  $0.3 \mu\text{m}$  wide. The density of states in the gap is shown in the inset. (b) 2D SIT shown in the inset having the following dimensions: source-drain distance is  $3.3 \mu\text{m}$ , source-gate distance is  $1 \mu\text{m}$ , gate width is  $2 \mu\text{m}$ , gate-to-gate distance is  $4 \mu\text{m}$ , thickness of gate is  $0.3 \mu\text{m}$ . The density of states in the gap is the same as inset of (a).

devices. Both analysis and numerical experiments have shown that slowing down or even failure of convergence may occur if Gummel's method is not properly extended to the a-Si:H case. The essential parameter is identified as the midgap density of states. This adapted Gummel method, we believe, will be of great utility in other amorphous-semiconductor-based device studies. The detailed simulation results of a-Si:H SIT are to be published elsewhere.

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- M. Kemp**, photograph and biography not available at the time of publication.
- C. G. Tannous**, photograph and biography not available at the time of publication.
- M. Meunier (A'85)**, photograph and biography not available at the time of publication.