Proceedings of the 4th International Conference on the Numerical Analysis of Semiconductor Devices and Integrated Circuits

NASECODE IV

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Proceedings of the Fourth International Conference on the Numerical Analysis of Semiconductor Devices and Integrated Circuits

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PREFACE

The Fourth International Conference on the Numerical Analysis of Semiconductor Devices and Integrated Circuits, NASECODE IV, was held in Trinity College, Dublin, Ireland, from 19th to 21st June 1985 under the auspices of the Numerical Analysis Group. This conference was the fourth in the NASECODE series; it was attended by 130 delegates from 27 countries.

The aim of these international conferences is the fostering of a fruitful exchange of ideas between electronic engineers on the one hand and numerical analysts on the other who are using existing and developing new computer codes for the computational modelling of semiconductor processes, devices and integrated circuits. As on previous occasions the industrial sector was strongly represented and it remains our goal to ensure that the topics discussed are relevant to the needs of industry. This policy guarantees that the scientific and technical material presented is not only intellectually challenging but is also of practical importance. The next conference in the series, NASECODE V, will be held in Dublin from 17th to 19th June, 1987.

Two additional events were held in association with NASECODE IV. The first of these was a short course which was held on 17th and 18th June 1985. The Lecture Notes, entitled "New Problems and New Solutions for Device and Process Modelling" are published in a companion volume to this. The second event was a workshop on the topic "An Introduction to Circuit-Level Simulation for VLSI Design and Verification". This was held on 24th and 25th June. There are no publications available from this event. However it has been decided to organise a short course and to encourage papers on this and related topics on the occasion of the NASECODE V Conference.

The present volume contains the full texts of the 10 keynote papers and 68 shorter papers. The papers were received from the authors in camera-ready form. The choice of this format has made possible publication within eight weeks of the event.

It is most gratifying to see the growing interst worldwide in the NASECODE Conferences. In particular, many new faces appeared at NASECODE IV and there was a marked increase in the number of contributed papers. It is a pleasure to thank the participants, the speakers, the sponsors and the many people behind the scenes, all of whom contributed generously to the success of this Conference.

Dublin, June 1985 J.J.H. Miller

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HFIELDS: a Highly Flexible 2–D Semiconductor–Device Analysis Program

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1. Introduction

HFIELDS (*Hybrid FInite–ELement Device Simulator*) is a general–purpose, two–dimensional, semiconductor–device analysis program developed at the University of Bologna, which does not impose any restriction on device geometry. The program employs a triangular–element mesh which can easily conform to irregularly shaped boundaries, and supports a variety of boundary conditions to simulate ideal and resistive ohmic contacts, Schottky–barrier junctions, gates and floating gates, and reflective boundaries.

At the user's option, the program can solve either Poisson's equation only, or Poisson's and one carrier continuity equation, or Poisson's and both carrier continuity equations, so that the numerical effort can be taylored to the specific problem at hand.

HFIELDS supports the most important physical effects affecting device performance, such as bandgap narrowing due to heavy doping, SRH and Auger recombination, impact ionization, and a number of mobility models with various degrees of sophistication and accuracy. Consequently, an extremely wide variety of silicon devices, both MOS and bipolar, can be realistically and efficiently simulated.

Up to ten semiconductor and insulator regions are allowed by HFIELDS, each of which can be a simply– or multiply–connected domain. For each region, a different set of models and model parameters may be defined; the program handles therefore insulator–semiconductor, semiconductor–semiconductor, and insulator–insulator interfaces.

Structure generation is accomplished via a user–friendly, interactive preprocessor, called BRÜNNHILDE, by which device geometry, impurity concentration, boundary conditions, physical models and parameters, and commands are defined and made available to the solver. The input preprocessor is completely menu–driven. An option to the use of BRÜNNHILDE is represented by IDAS, a process–oriented input preprocessor developed at SGS [Lombardi *et. al.*, 1985]. IDAS, in turn, makes use of the DAMSEL organization developed at CNET [Belhaddad *et. al.*, 1985].

Mesh generation can be performed either automatically or interactively, via a module called ATMOS (*Automatic Triangular–Mesh generation and Optimization System*), fully interfaced to BRÜNNHILDE and IDAS. Criteria for mesh refinement are related to the curvature of the boundary, doping gradient, and inversion layers. If the resulting mesh is not adequate to the specific needs of the user, the latter can interactively define windows on the device cross section, and force horizontal and/or vertical refinement of the grid.

This work is organized as follows: next section illustrates the basic semiconductor equations, the physical models and the boundary conditions supported by the program. Section 3 is devoted to the numerical techniques, with regard to the problem of discretization and to the solution method. Section 4 illustrates mesh generation, and section 5 provides the description of results obtained in the simulation of a Schottky–clamped BJT.

2. Physical Model

In its present version, the program solves the basic semiconductor equations in steady state, i. e.

$$\mathrm{div}\,(\epsilon_s\,\mathrm{grad}\varphi) = -q\,(p - n + N_D - N_A) \tag{1,a}$$

$$\mathrm{div}(\mathbf{J}_n/q) = (R - G) \tag{1,b}$$

$$-\mathrm{div}(\mathbf{J}_p/q) = (R - G), \tag{1,c}$$

where the current densities $\mathbf{J}_n$ and $\mathbf{J}_p$ are classically expressed as

$$\mathbf{J}_n = -q\mu_n n\,\mathrm{grad}(\varphi + \Delta\psi_c) + qD_n\,\mathrm{grad}n \tag{2,a}$$

$$\mathbf{J}_p = -q\mu_p p\,\mathrm{grad}(\varphi - \Delta\psi_v) - qD_p\,\mathrm{grad}p. \tag{2,b}$$

In eqns. (1), (2), the various symbols are given the usual meaning; $\Delta\psi_c$ and $\Delta\psi_v$ represent the conduction and valence band–edge shift due to heavy doping. As only the total bandgap

narrowing $\Delta\psi_G = \Delta\psi_c + \Delta\psi_v$ can be experimentally determined from either optical or electrical measurements, we assume, as it is customary, $\Delta\psi_c = \Delta\psi_v = \Delta\psi_G/2$.

Bandgap narrowing $\Delta\psi_G$ is assumed to follow Slotboom and De Graaf's expression

$$\Delta E_G = q\,\Delta\psi_G = E_{BGN}\left[\ln(N_i/N_{BGN}) + \left(\ln^2(N_i/N_{BGN}) + C_{BGN}\right)^{1/2}\right], \tag{3}$$

where $N_i = N_D + N_A$ is the total impurity concentration, and E_{BGN}, N_{BGN}, and C_{BGN} are suitable parameters [Slotboom and De Graaf, 1976].

The net recombination rate on the RHS of eqns. (1,b), (1,c) comprises several physical effects, i. e. SRH and Auger recombination and impact ionization. Thus,

$$(R-G) = (R-G)_{SRH} + (R-G)_{AUG} - G_{IMP}, \tag{4}$$

where

$$(R-G)_{SRH} = \frac{np - n_{ie}^2}{\tau_{p0}(n+n_1) + \tau_{n0}(p+p_1)}, \tag{5,a}$$

$$(R-G)_{AUG} = (c_n n + c_p p)\left(np - n_{ie}^2\right), \tag{5,b}$$

$$G_{INP} = \alpha_n n v_n + \alpha_p p v_p. \tag{5,c}$$

In eqn. (5,a), $n_1 = n_{ie}\exp[(E_t - E_i)/kT]$ and $p_1 = n_{ie}\exp[(E_i - E_t)/kT]$, E_t being the trap energy. In eqn. (5,c), v_n and v_p represent the electron and hole velocities, respectively, and α_n, α_p are the electron and hole ionization coefficients. In HFIELDS, Chynoweth's expressions (1958) are used for α_n, α_p, i. e.

$$\alpha_n = A_n \exp(-b_n/E_{ln}) \tag{6,a}$$

$$\alpha_p = A_p \exp(-b_p/E_{lp}), \tag{6,b}$$

where $E_{ln} = \mathbf{E}\bullet\mathbf{J}_n/|\mathbf{J}_n|$ and $E_{lp} = \mathbf{E}\bullet\mathbf{J}_p/|\mathbf{J}_p|$; default values for the above parameters are taken from Van Overstraeten and De Man (1970).

HFIELDS supports several mobility models which incorporate an increasing number of scattering mechanisms: first, mobility is expressed vs effective doping N_{ie} according to Caughey and Thomas (1967)

$$\mu_0 = \mu_{min} + \frac{\mu_{max} - \mu_{min}}{1 + (N_{ie}/N_{ref})^{\alpha}}, \tag{7}$$

where the temperature dependence of the above parameters is chosen from Arora et. al. (1982). In eqn. (7), N_{ie} may account for electron–hole scattering according to Engl and Dirks (1981):

$$N_{ie} = \alpha_{eh} N_i + (1-\alpha_{eh})(n+p). \tag{8}$$

Eqn. (8) is appropriate for bipolar devices, and the correction becomes significant in high–injection conditions. For MOSFET's, where no appreciable electron–hole scattering occurs, $N_{ie} = N_i$.

Next, mobility dependence upon the quasi–Fermi potential gradient F is accounted for by means of the Caughey and Thomas expression

$$\mu = \frac{\mu_0}{\left[1 + \left(\frac{\mu_0 F}{v_{sat}}\right)^{\beta}\right]^{1/\beta}}, \tag{9}$$

where the saturation velocity and its temperature dependence are taken from [Canali et. al., 1975].

In MOSFET's, surface scattering is an additional limiting factor for mobility; this effect is accounted for by HFIELDS following Yamaguchi (1983):

$$\mu_s = \mu_0 (1 + \alpha_s E_t)^{-1/2}, \tag{10}$$

where E_t is the component of the electric field normal to current flow, and μ_s, rather than μ_0, is used in eqn. (9).

As a possible alterntive, HFIELDS supports the Gummel–Thornber model for mobility (1980), i. e.

$$\mu = \frac{\mu_0}{\left[1 + \left(\frac{\mu_0 F}{u_l}\right)^2 \left(G + \frac{\mu_0 F}{u_l}\right)^{-1} + \left(\frac{\mu_0 F}{v_{sat}}\right)^2\right]^{1/2}}, \tag{11}$$

where

$$\mu_0 = \mu_L \left[1 + N_{ic}/(N_{ic}/S + N_{ref})\right]^{-1/2}. \tag{12}$$

In eqns. (11), (12), u_l is the acoustic–phonon longitudinal velocity, and μ_L is the lattice mobility. For MOSFET's, eqn. (10) is again accounted for, and μ_s, rather than μ_0, is used in eqn. (11).

When dielectric regions are active parts of the device to be simulated, only Poisson's equation is solved in the insulator, i. e.

$$\mathrm{div}\,(\epsilon_i\,\mathrm{grad}\varphi) = -\rho_i,$$

where ρ_i is the insulator–trapped charge. At the insulator–semiconductor interface, continuity of the electric potential is assumed, along with the following boundary conditions

$$(\mathbf{D}_s - \mathbf{D}_i) \bullet \hat{\imath}_n = Q_{it} \tag{13,a}$$

$$\mathbf{J}_n \bullet \hat{\imath}_n = q\,(R - G)_s \tag{13,b}$$

$$\mathbf{J}_p \bullet \hat{\imath}_n = -q\,(R - G)_s, \tag{13,c}$$

where $\mathbf{D}_s$ and $\mathbf{D}_i$ represent the electric displacement vectors at the semiconductor– and insulator–side of the interface, Q_{it} is the interface–trapped charge, and $(R - G)_s$ is the net surface recombination rate. Also, $\hat{\imath}_n$ is a normal versor oriented toward the semiconductor.

HFIELDS supports several types of boundary conditions, to account for the specific needs of different devices: ideal ohmic contacts, resistive ohmic contacts, Schottky contacts, gates, floating gates, and reflective boundaries.

At ideal ohmic contacts, the following boundary conditions are imposed:

$$\varphi_c = V_c + (kT/q)\sinh^{-1}(N/2n_{ic}) \tag{14,a}$$

$$n_c = \sqrt{\frac{N^2}{4} + n_{ic}^2} + \frac{N}{2} \tag{14,b}$$

$$p_c = \sqrt{\frac{N^2}{4} + n_{ic}^2} - \frac{N}{2}, \tag{14,c}$$

where $N = N_D - N_A$ is the net impurity concentration and subscript c stems from contact.

At resistive ohmic contacts, eqn. (14,a) is modified as follows

$$\varphi_c = V_c + (kT/q)\sinh^{-1}(N/2n_{ic}) - \rho_c \mathbf{J} \bullet \hat{\imath}_n, \tag{15}$$

where $\hat{\imath}_n$ is an inward–oriented normal versor; eqns. (14,b) and (14,c), instead, are left unmodified.

At Schottky–barrier junctions, the following conditions, arising from the thermionic–diffusion theory, are imposed:

$$\varphi_c = V_c - \Phi_B + (kT/q)\,\ln(N_c/n_{ic}) \tag{16,a}$$

$$\mathbf{J}_n \bullet \hat{\imath}_n = q v_n^T (n_c - n_o) \tag{16,b}$$

$$\mathbf{J}_p \bullet \hat{\imath}_n = -q v_p^T (p_c - p_o), \tag{16,c}$$

where Φ_B is the barrier height, v_n^T and v_p^T are the thermionic emission velocities, defined as

$$v_n^T = A_n^* T^2/qN_c \tag{17,a}$$

$$v_p^T = A_p^* T^2/qN_v, \tag{17,b}$$

A_n^*, A_p^* being the Richardson constants for electrons and holes, and n_0, p_0 the equilibrium carrier concentrations at the junction, i. e.

$$n_0 = n_{ic}\,\exp(q\varphi_0/kT) \tag{18,a}$$