COMPUTER ANALYSIS OF SEMICONDUCTOR STRUCTURES

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Introduction

Since the pioneering work of KENNEDY and O'BRIEN [1] a lot of work has been done on the two-dimensional numerical analysis of semiconductor structures. Now 10—20 such programs are working all over the world. The significance of the two-dimensional analysis is the following: 1. better understanding of the physical processes, 2. refinement of the network models, 3. preliminary control of new structures. Making use of the experiences of a Thesis [2] made under our guidance, we have developed a user-oriented system leaving much freedom of choosing the boundary conditions (optional poligonal semiconductor with optional number of ohmic or rectifying contacts, electrode over oxide layer and insulating boundary).

Governing equations, boundary conditions

The following normed equations describe the steady stream problem (on the normalization see [3]):

$$\operatorname{div}\left(\mu_{p}e^{-\varphi}\operatorname{grad}e^{\varphi_{p}}\right) = R , \qquad (1)$$

div
$$(\mu_n e^{\varphi} \operatorname{grad} e^{-\varphi_n}) = R$$
, (2)

$$\Delta \varphi = -e^{\varphi_p - \varphi} + e^{\varphi - \varphi_n} + N , \qquad (3)$$

where φ is the electrical potential, φ_p and φ_n are the hole and electron Fermi potentials, respectively, μ_p and μ_n are the hole and electron mobilities, respectively, R is the recombination rate, N is the doping concentration.

The boundary conditions are (-0 and + 0 refer to metal contact and to semiconductor, respectively)

ohmic contact: $\varphi_n(+0) = \varphi(-0), \ \varphi_n(+0) = \varphi(-0),$

 $\varphi(+0) = \varphi(-0) + \ln N(+0)$, the upper sign refers to donor doping, the lower to acceptor doping,

rectifying contact: $\varphi_p(+0) = \varphi(-0)$, $\varphi_n(+0) = \varphi(-0)$, $\varphi(+0) = \varphi(-0) + U_s$, U_s is a constant characteristic of the contact, insulating boundary: $\partial \varphi_p / \partial v = 0$, $\partial \varphi_n / \partial v = 0$ or φ prescribed,

where v is the surface normal.

The foregoing nonlinear, elliptic, partial system of differential equations can be solved only numerically. Let us examine a picked-up detail of the far reaching problems, deducing in a unified manner the difference schemes of the current density appeared in the literature.

Difference schemes of the current density

 $e^{-\varphi_n}$ is known to be a potential belonging to the field $-J_n/\mu_n e^{\varphi}$, i.e., for an arbitrary path between A and B

$$e^{-\varphi_n(A)} - e^{-\varphi_n(B)} = -\int_A^B \frac{\overline{J_n}}{\mu_n e^{\varphi}}.$$
(4)

If the current density is constant

$$J_n = -\frac{e^{-\phi_n(A)} - e^{-\phi_n(B)}}{\int\limits_A \frac{1}{\mu_n} e^{-\phi} dl}$$
(5)

In formula (5) the denominator can be evaluated at different accuracies. leading to the different expressions for the current density appeared in the literature.



Fig. 1. Computation of the current density

For the sake of survey only the electrical potential is indicated in the grid of Fig. 1. Only the component $J_{i+\frac{1}{2},j}$ of the electron current is dealt with, therefore the constant subscript j is omitted.

1.
$$\mu_n = \mu_{i+\frac{1}{2}} = \text{const.}, \ \varphi = (\varphi_i + \varphi_{i+1})/2 = \text{const.}, \text{ then}$$

$$J_{i+\frac{1}{2}} = \mu_{i+\frac{1}{2}} e^{(\varphi_i + \varphi_{i+1})/2} \frac{e^{-\varphi_{ni+1}} - e^{-\varphi_{ni}}}{h_{i+1}},$$
(6)

the same as the formula by VANDORPE [4] containing "space-dependent normalization".

2. Evaluation of the integral in the denominator by trapezoid rule

$$J_{i+\frac{1}{2}} = \frac{e^{-\varphi_{ni+1}} - e^{-\varphi_{ni}}}{\frac{h_{i+1}}{2} \left(\frac{1}{\mu_{ni}} e^{-\varphi_{i}} + \frac{1}{\mu_{ni+1}} e^{-\varphi_{i+1}}\right)}$$
(7)

Disadvantage of formulas (6) and (7) is to cause a great error for a high voltage between two grid points.

3. Let us approximate $1/\mu_n(x)$ and $\varphi(x)$ between two grid points by linear function

$$\frac{1}{\mu_n(x)} = \frac{1}{\mu_{ni}} + \frac{\frac{1}{\mu_{ni+1}} - \frac{1}{\mu_{ni}}}{h_{i+1}} x, \qquad (8)$$

$$\varphi(x) = \varphi_i + \frac{\varphi_{i+1} - \varphi_i}{h_{i+1}} x.$$
(9)

Evaluating the integral results in:

•

$$J_{i+\frac{1}{2}} = \left(e^{-\varphi_{ni+1}} - e^{-\varphi_{ni}}\right) \left| \frac{h_{i+1}}{\varphi_{i} - \varphi_{i+1}} \left[e^{-\varphi_{i+1}} \left(\frac{1}{\mu_{ni+1}} - \frac{1}{\mu_{ni}} - \frac{1}{\mu_{ni}} \right) - \frac{1}{\varphi_{i} - \varphi_{i+1}} \right) - \frac{1}{\varphi_{i} - \varphi_{i+1}} \right] - e^{-\varphi_{i}} \left(\frac{1}{\mu_{ni}} - \frac{1}{\mu_{ni+1}} - \frac{1}{\mu_{ni}} - \frac{1}{\mu_{ni}} \right) \right].$$

$$(10)$$

To our knowledge the result (10) has not yet been used in the literature. In the special case where the mobility between two grid points is not linear but

constant, i.e. $\mu_{ni+1} = \mu_{ni} = \mu_{ni+\frac{1}{2}}$, then (10) transformed to the formula of SCHARFETTER and GUMMEL [5]. (5) shows also the potential not to be approximable by parabola as a further refinement, because in this case the integral in the denominator cannot be expressed in closed form.

Functional description of the program system

The system consists of two main functional units, which can be used either independent or joint. The functions of the two main programs are

a) *field analysis program:* the program determines the steady stream field of the given semiconductor structure,

b) post processor program: it processes in graphical and tabular form the results of the field analysis program.

A run of the program needs three data sets, two being included in public libraries (layout structures, technological data) and one storing the results of the field analysis.



Fig. 2a. Data input



Fig. 2b. Field analysis



233



Fig. 3. Equipotential lines of a MESFET

In the flow chart the different data sets are named as follows:

data set A: technological parameters

data set B: layout structures

data set C: storing of the results of field analysis for post processing.

Layout and technological parameters of the structure can be given directly on punched cards instead of public libraries.

The functional flow chart of the system is seen in Fig. 2.

As an example, the equipotential lines of the electrical potential of a MES-FET is seen in Fig. 3.

Summary

A program system is presented, suitable for the two-dimensional numerical analysis of the steady stream field of semiconductor structures. The program system is user-oriented and leaves a great freedom in choosing the shape of the semiconductor and the boundary conditions. The different finite difference formulae of the current density are analysed in detail. The flow chart of the program system is presented and some results are shown.

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