A Method for Unified Treatment of Interface Conditions Suitable for Device Simulation

T. Simlinger, M. Rottinger, and S. Selberherr
Institute for Microelectronics, TU Vienna
Gusshausstrasse 27–29, A-1040 Vienna, Austria
http://www.iue.tuwien.ac.at/

Abstract—A method is presented which allows for a unified treatment of interface conditions covering also both extreme cases, Dirichlet and Neumann boundary conditions. This unified treatment is especially useful if the type of the interface condition depends on the internal state of the device. The method is applied to a heterojunction interface where thermionic fieldemission and tunneling is assumed.

I. INTRODUCTION

Simulation has become a standard supplement for the development of new semiconductor devices. Often the characteristics of these devices are determined by physical effects for which the development of suitable models is difficult. Several of these effects, such as carrier heating or quantum phenomena, gain influence on the device characteristics when the feature size falls below a certain limit and the impact of interfaces on bulk behavior can not be neglected any more. Thus, proper interface modeling plays an important role for device simulation.

Especially modeling the electron and hole current across interfaces has been found to be a complex task and a large number of models for different types of interfaces have been proposed [8][3][2][9]. For device simulation the interface type is automatically detected by analyzing the device structure or is explicitly defined as an input parameter. This method works well as long as the interface type does not depend on the internal state of the device. For instance the thermionic emission model is commonly used for modeling the current across heterojunctions of compound semiconductors. This model can be extended to the thermionic field-emission model to account for tunneling effects through the heterojunction barrier.

If the tunneling effect becomes more and more dominating, the model will no longer determine the current across the interface. Instead the model establishes a direct relationship between the carrier concentrations on both sides of the interface. Thus, sloppily speaking, the interface type changes from a more Neumann boundary condition to a more Dirichlet boundary condition. Dirichlet boundary conditions require numerical methods which are different to methods for Neumann boundary conditions. If

an interface model uses a numerical method for Neumann boundary conditions and the interface type changes to a more Dirichlet type the condition of the linear system to solve is poor and deteriorates the convergence behavior. In this work a unified treatment of interface models is proposed which allows for changing interface types without negative influence on convergence.

II. THE NEW METHOD

The new method for specifying interface conditions is capable of handling all types of boundary conditions used in device simulation, including the extreme cases of Dirichlet (1) and Neumann (2) boundary conditions.

$$u = a \tag{1}$$
$$\vec{n} \cdot \mathrm{grad}\, u = b \tag{2}$$

The unified treatment of interface conditions is demonstrated for modeling the current flow across a heterojunction interface (see Fig. 1b, c) [4]:

$$J_\perp = \alpha\,(e_\mathrm{b}) \cdot q \cdot \left[v_2 \cdot n_2 - \frac{m_2}{m_1} \cdot v_1 \cdot n_1 \cdot \exp\left(-e_\mathrm{b}\right) \right],$$

$$v_i = \sqrt{\frac{k_\mathrm{B} \cdot T_i}{2 \cdot \pi \cdot m_i}}, \quad e_\mathrm{b} = \frac{\Delta E_C \left(-\frac{\partial \psi}{\partial n}\right)}{k_\mathrm{B} \cdot T_1}. \tag{3}$$

The value of the factor α depends on the shape of the energy barrier and the physical effects taken into account. For a simple thermionic emission model α is equal to 1. v_i is the thermionic emission velocity and e_b the effective barrier height of the heterojunction. $\Delta E_C \left(-\frac{\partial \psi}{\partial n}\right)$ is the difference of the conduction band edge energies which depends on the normal component of the electric field.

When a finite box discretization scheme is used, one obtains for the discretization point i on the interface (see Fig. 1a)

$$\text{Box } i_1 : \quad \sum_{j_1} J_{j_1} = +J_{i\perp}, \tag{4}$$

$$\text{Box } i_2 : \quad \sum_{j_2} J_{j_2} = -J_{i\perp}. \tag{5}$$

Fig. 2. One-dimensional discretization of the continuity equation across an interface. The boundary values n_1 and n_4 are fixed (Dirichlet boundary condition). For the current across the interface the thermionic field-emission model (3) is used.
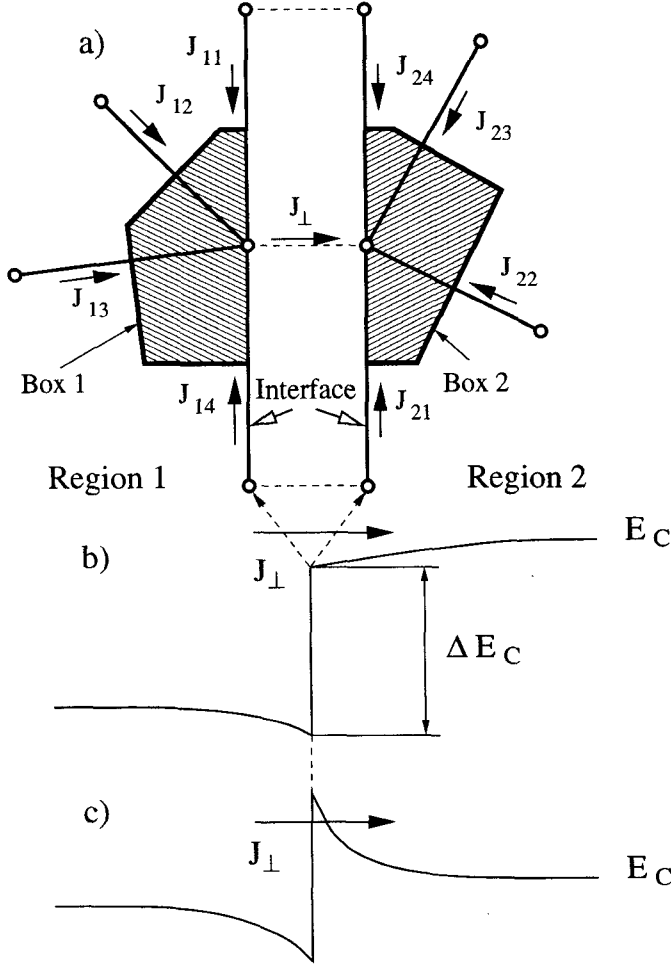
Fig. 1. Finite box discretization (a), current flow across a heterojunction interface without (b) and with (c) tunneling.

The subscripts 1 and 2 denote quantities associated to regions 1 and 2, respectively.

If tunneling is negligible, the current flow is suitably approximated by the thermionic emission model (3). However, very often tunneling must be taken into account, e.g., by a field-dependent barrier height lowering. Tunneling as well as carrier heating can reduce the effective barrier height significantly, and in its limit it approaches zero. Thus, large values of α can occur as $\lim_{e_b \to 0} \alpha(e_b) = \infty$. Since $J_\perp$ must remain finite, this limit simply implies that the boundary condition changes to Dirichlet type:

$$\lim_{e_b \to 0} \frac{1}{\alpha} J_{i\perp} = 0 = f(n_1, n_2),$$

$$f(n_1, n_2) = q \cdot \left[v_2 \cdot n_2 - \frac{m_2}{m_1} \cdot v_1 \cdot n_1 \right]. \quad (6)$$

Hence, a low perpendicular component of the electric field on the interface and the absence of carrier heating result in a Neumann type condition for current flow across
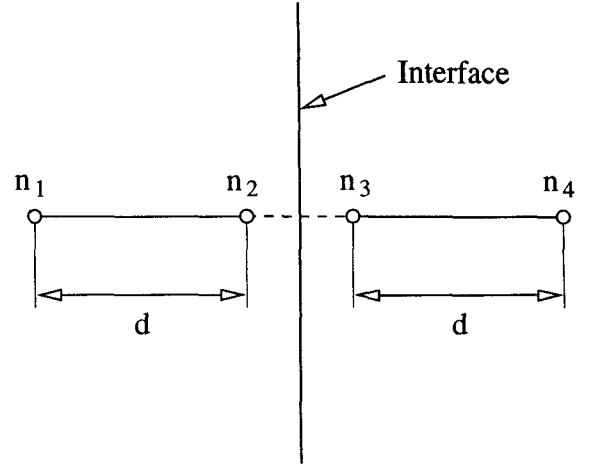
the interface, whereas for increasing electric field or carrier temperature the interface model (3) determines the carrier concentration itself rather than the current flow across the interface.

Large values of α which occur for effective barrier heights near zero increase the spectral condition number of the system matrix [1][7], as will be demonstrated. For iterative linear solvers the spectral condition number is a measure for the accuracy of the solution:

$$\kappa_s = \frac{|\lambda|_{\max}}{|\lambda|_{\min}}. \quad (7)$$

$|\lambda|_{\max}$ and $|\lambda|_{\min}$ are the eigenvalues with maximum and minimum magnitude of the system matrix. The larger the value of κ_s the poorer is the condition of the system matrix.

Considering the one-dimensional discretization of the continuity equation (see Fig. 2)

$$J = q \cdot D \cdot \frac{\partial n}{\partial x}, \quad (8)$$

and assuming the electrostatic potential and dielectric flux as constant at the heterojunction, one obtains for n_2 and n_3 the equations

$$\begin{pmatrix} -\alpha \cdot \dfrac{m_3}{m_2} \cdot v_2 \cdot \exp(-e_b) - \dfrac{D}{d} & +\alpha \cdot v_3 \\ +\alpha \cdot \dfrac{m_3}{m_2} \cdot v_2 \cdot \exp(-e_b) & -\alpha \cdot v_3 - \dfrac{D}{d} \end{pmatrix} \cdot \begin{pmatrix} n_2 \\ n_3 \end{pmatrix} =$$

$$= \begin{pmatrix} -\dfrac{D}{d} \cdot n_1 \\ -\dfrac{D}{d} \cdot n_4 \end{pmatrix}. \quad (9)$$

For the interface current (3) has been inserted. n_1 and n_4 are the fixed values on the left and the right boundary (Dirichlet boundary condition).

If α is large, the eigenvalues of (9) read

$$\lambda_1 = -\alpha \cdot \left(v_3 + \frac{m_3}{m_2} \cdot v_2 \cdot \exp(-e_b) \right) \quad (10)$$

$$\lambda_2 = -\frac{D}{d}. \quad (11)$$

Thus,

$$\kappa_s \propto \alpha \quad (12)$$

and, therefore, for large α the spectral condition of the system matrix will be poor. Thus, if the internal state of a device results in a large value of α the solver cannot compute the solution of the linear system with sufficient accuracy. The result will be an increase of iteration steps for the Newton scheme, if convergence can be achieved at all.

This problem can be alleviated by transforming the linear system (9) as follows. Adding the second equation to the first one and scaling the second equation with $\frac{1}{\alpha}$ results in the new system

$$\begin{pmatrix} -\dfrac{D}{d} & -\dfrac{D}{d} \\ +\dfrac{m_3}{m_2} \cdot v_2 \cdot \exp(-e_b) & -v_3 - \dfrac{1}{\alpha} \cdot \dfrac{D}{d} \end{pmatrix} \cdot \begin{pmatrix} n_2 \\ n_3 \end{pmatrix} =$$

$$= \begin{pmatrix} -\dfrac{D}{d} \cdot (n_1 + n_4) \\ -\dfrac{1}{\alpha} \cdot \dfrac{D}{d} \cdot n_4 \end{pmatrix}. \quad (13)$$

This system matrix has the eigenvalues

$$\lambda_{1,2} = -\frac{1}{2} \cdot \left(v_3 + \frac{D}{d} \right) \pm \quad (14)$$

$$\pm \sqrt{\frac{1}{4} \cdot \left(v_3 - \frac{D}{d} \right)^2 - \frac{m_3}{m_2} \cdot v_2 \cdot \exp(-e_b)},$$

hence, κ_s does not longer depend on α. The strong influence of the internal state of the device on the spectral condition of the equation system has been eliminated.

Applying the above transformation to the two-dimensional situation, the equations for box i_1 and i_2 can be rewritten such as

$$\text{Box } i_2: \quad \sum_{j_2} J_{j_2} + \sum_{j_1} J_{j_1} = 0, \quad (15)$$

$$\text{Box } i_1: \quad \sum_{j_1} J_{j_1} = J_{i\perp}. \quad (16)$$

Equation (15) is Kirchhoff's law for the compound of box i_1 and i_2 (i.e., the sum of (4) and (5)) and determines
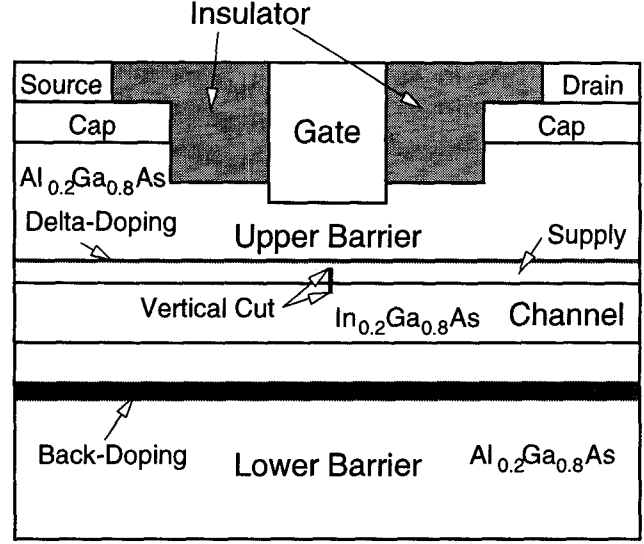

Fig. 3. Schematic cross section of the simulated delta-doped pseudomorphic double-heterojunction HEMT. The region of the vertical cut of Fig. 4 and Fig. 5 is marked.

electron concentration n_2, (16) does the same for box i_1 and determines n_1. The problem of α becoming large can be easily solved by scaling (16) with $\frac{1}{\alpha}$ as proposed for the one-dimensional case:

$$\tilde{\alpha} \cdot \sum_{j_1} J_{j_1} = f(n_1, n_2, e_b), \quad \tilde{\alpha} = \frac{1}{\alpha}. \quad (17)$$

For $\lim_{e_b \to 0} \tilde{\alpha}(e_b) = 0$ follows $f(n_1, n_2) = 0$ which is equivalent to the Dirichlet boundary condition

$$n_1 = n_2 \cdot \left(\frac{m_1}{m_2} \right)^{\frac{3}{2}} \cdot \left(\frac{T_2}{T_1} \right)^{\frac{1}{2}}. \quad (18)$$

Instead of large values of α the simulator has now simply to cope with small values of $\tilde{\alpha}$. Furthermore, the spectral condition of the system matrix is not deteriorated by large values of α.

III. EXAMPLE

As an example a delta-doped pseudomorphic double-heterojunction HEMT (high electron mobility transistor) has been simulated with MINIMOS-NT [5][6] using a hydrodynamic model. Fig. 3 shows a schematic cross section of the simulated device. The energy flux across the heterojunction interface was modeled by

$$S_\perp = -2 \cdot \beta \cdot \left[\Lambda_2 - \frac{m_2}{m_1} \cdot \Lambda_1 \cdot \exp(-e_b) \right],$$

$$\Lambda_i = k_B \cdot T_i \cdot v_i \cdot n_i,$$

$$S_2 = S_1 + \frac{k_B \cdot T_1}{q} \cdot e_b \cdot J_\perp. \quad (19)$$

175
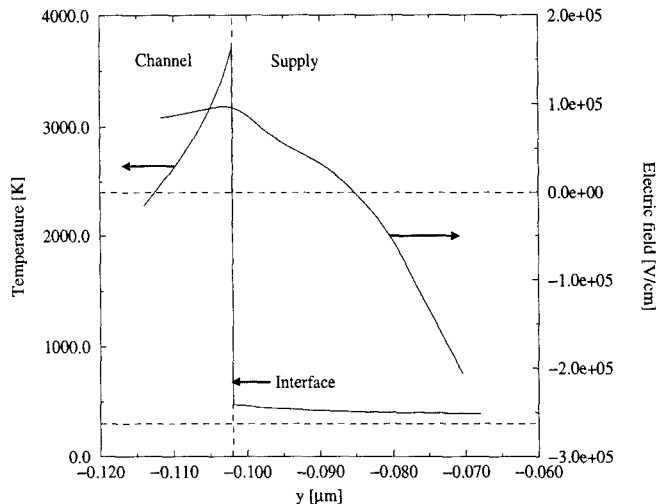
Fig. 4. Carrier temperature and electric field along a vertical cut across the channel–supply interface of a pseudomorphic HEMT.

Fig. 5. Electron concentration and current density along the same vertical cut as in Fig. 4.

Similar to α in (3) the value of the factor β depends on the energy barrier and the physical models taken into account.

The bias point was chosen in such a way that the carriers heat up considerably in the channel and the effective barrier height is close to zero. Fig. 4 shows the electron temperature and the electric field along a vertical cut across the heterojunction. Normally, the carrier concentration inside the channel is several orders of magnitude higher than in the supply region. For the example shown the situation is reversed as the carrier temperature in the channel exceeds the temperature in the supply region (18). Therefore a large number of electrons has sufficient kinetic energy to surmount the barrier at the heterojunction and reach the supply region (real-space transfer). Although the electron concentration in the channel is much lower than in the supply a considerable amount of the current is conducted in the channel due to the much higher mobility in the channel. The electron concentration and the current density are shown in Fig. 5. This example can only be simulated with our new method.

IV. CONCLUSION

The proposed method for a unified treatment of interface conditions is very useful for simulation of generic semiconductor devices and is an elegant way to handle bias dependent interface condition types. Furthermore, no distinction has to be made between heterojunction interfaces and interfaces where regions with identical material properties are joined. By transforming the equations describing the interface conditions the strong influence of the internal state of the device on the spectral condition of the equation system can be eliminated.
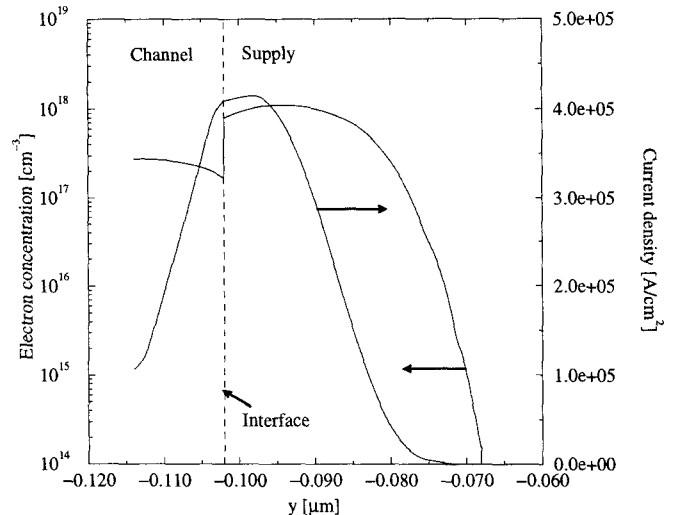
ACKNOWLEDGMENT

REFERENCES

[1] GOLUB, G.H., AND VAN LOAN, C.F. *Matrix Computations*, second ed. John Hopkins University Press, 1989.

[2] GRUPEN, M., HESS, K., AND SONG, G.H. Simulation of Transport over Heterojunctions. In Proc: *Simulation of Semiconductor Devices and Processes* (Konstanz, 1991), W. Fichtner and D. Aemmer, Eds., vol. 4, Hartung-Gorre, pp. 303–310.

[3] MOTTET, S., AND VIALLET, J.E. Thermionic Emission in Heterojunctions. In Proc: *Simulation of Semiconductor Devices and Processes* (Bologna, 1988), G. Baccarani and M. Rudan, Eds., vol. 3, Tecnoprint, pp. 97–108.

[4] SCHROEDER, D. *Modelling of Interface Carrier Transport for Device Simulation.* Springer, 1994.

[5] SIMLINGER, T., KOSINA, H., ROTTINGER, M., AND SELBERHERR, S. MINIMOS-NT: A Generic Simulator for Complex Semiconductor Devices. In Proc: *ESSDERC'95 - 25th European Solid State Device Research Conference* (Gif-sur-Yvette Cedex, France, 1995), H. de Graaff and H. van Kranenburg, Eds., Editions Frontieres, pp. 83–86.

[6] SIMLINGER, T., BRECH, H., GRAVE, T., AND SELBERHERR, S. Simulation of Submicron Double-Heterojunction High Electron Mobility Transistors with MINIMOS-NT. *IEEE Trans.Electron Devices 44*, 5 (1997), 700–707.

[7] VARGA, R.S. *Matrix Iterative Analysis.* Prentice-Hall, 1962.

[8] WU, C.M., AND YANG, E.S. Carrier Transport Across Heterojunction Interfaces. *Solid-State Electron. 22* (1979), 241–248.

[9] YANG, K., EAST, J.R., AND HADDAD, G.I. Numerical Modeling of Abrupt Heterojunctions Using a Thermionic-Field Emission Boundary Condition. *Solid-State Electron. 36*, 3 (1993), 321–330.