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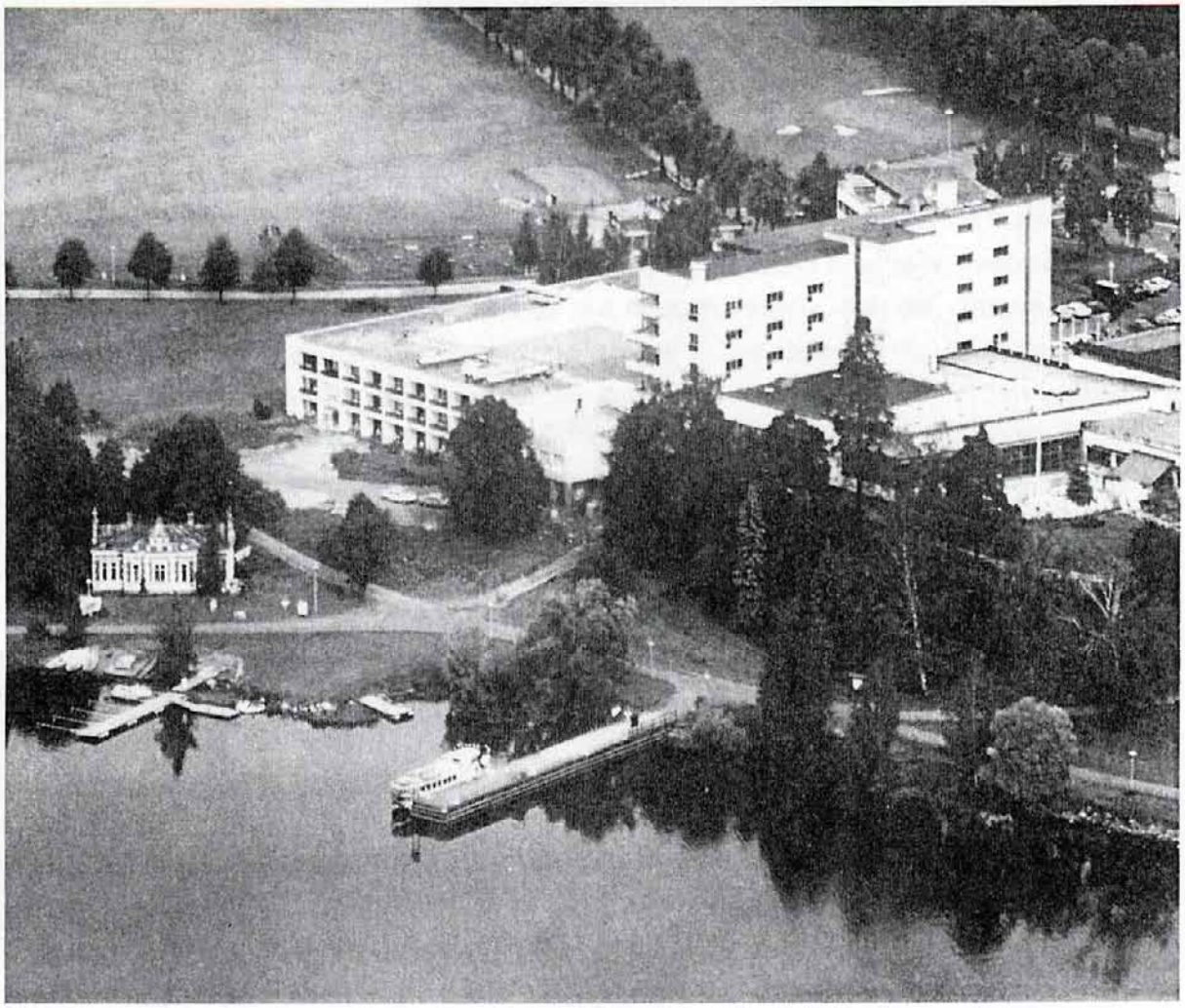

PROCEEDINGS

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QUANTUM MECHANICAL APPROACH FOR THE EXAMINATION OF THE PROPERTIES OF MOS INVERSION LAYERS IN p-TYPE SILICON [1]

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ABSTRACT

For a submicron MOS transistor having a channel length of approx. 1 μm and assuming an active depth of 1 μm, the number of doping ions is in the order of 10^4 for a width of 1 μm in case of a doping concentration of 10^{22} m^{-3}. In strong inversion the quantity of inversion carriers is in the same order. These numbers have initiated us to develop a new 3D Monte Carlo simulation method which apply the real number of carriers for simulating their real field, movement, flow etc. Strong efforts are taken to use the possible deepest "first principles" in the active region of the MOS transistor instead of any abstractions generally used by usual semiconductor device simulators. A new method is described for the calculation of the 3D potential distribution. A detailed discussion is given on the accuracy limiting conditions arising partly from the numerical solution methods *(linearization errors)* and partly from the quantum mechanical behaviour of the carriers (*Heisenberg relation).*

INTRODUCTION

Decreasing semiconductor device dimensions results in increasing importance of *Monte Carlo simulation* methods, because

1. It is very difficult to apply the *continuum view* for a device having free carriers in the order of only some thousands.
2. For such a *small number of free carriers* the up-to-date computing facilities are able to give a possibility to follow the history of each carrier by using only reasonable computer time.

SIMULATION PRINCIPLE

The main steps of the Monte Carlo simulation are the following [1]:

1. determination the *potential and field distributions* in the active region caused by the ionized impurities and carriers, with given external voltages
2. describing the *carrier movement* in the real space and momentum space, during a short time Δt,
3. simulating the the effect of various *scattering mechanisms* (only the surface, intervalley and intravalley mechanisms are meant here, since the impurity and carrier-carrier scatterings are inherently processed in our method by using the 'real' trajectories of the carrier motion).

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4. end point checking: if an almost stationary field, carrier density and energy distribution is reached, the simulation is finished for the given external voltages, Otherwise a Δt time increment is again applied and the whole process is repeated from step 1.

The channel region and a restricted part of the bulk is examined by the Monte Carlo method. Out of this region a classical approach is used. The boundaries of the active region are

(i) the source - channel metallurgical junction,
(ii) the channel - drain metallurgical junction,
(iii) an 'equilibrium' area between the channel and the bulk,
(iv) the Si/SiO_2 interface.

The 6 ellipsoid modell is used for determining the *conduction band structure* and the Airy function approximation is applied for describing the *subband energies* 2]. The *narrow channel effect* is not considered, because a structure broad enough is assumed in the y - direction. For the planes limiting the structure from the left and right sides either a periodic boundary condition or averaging can be applied. The *generation - recombination effects* are neglected. Because the electrons spend a short time in the channel region, only a few scatterings occur during their flight. The method correctly follows the flight of those carriers performing pure *ballistic transport* (flying unscattered from source to drain). The effect of Si/SiO_2 *interface states* can be taken into consideration either by an uniform charge sheet at the interface, or by elementary charges at discrete positions at the interface.

CARRIER BEHAVIOUR

The motion of carriers in the real space is described by the *general laws of motion* (the Newtonian laws), assuming a driving force acting to the carrier

$$\mathbf{F}(\mathbf{r}(t),\ t) = \pm\, q\ \mathbf{E}(\mathbf{r}(t),\ t) \tag{1}$$

where the positive sign is valid for holes and the negative for electrons.

During a short flight time Δt for unscattered carriers the momentum change is given by

$$\Delta \mathbf{p} = \int_t^{t+\Delta t} \mathbf{F}(\mathbf{r}(t'),\ t')\ dt' \tag{2}$$

and the change in space coordinates is given by

$$\Delta \mathbf{r} = \int_t^{t+\Delta t} \mathbf{m}^{-1}\mathbf{p}(t')\ dt' \tag{3}$$

The velocity of the particle is related to the momentum by

$$\mathbf{v}(\mathbf{r}(t),\ t) = m^{-1}\mathbf{p}(\mathbf{r}(t),\ t) \tag{4}$$

where m^{-1} is the reciprocal effective mass tensor.

DETERMINATION OF THE POTENTIAL DISTRIBUTION

The potential distribution in semiconductor structures usually is determined by numerical solution of the Poisson equation

$$\text{div grad}\ \psi = \frac{q}{\varepsilon}\left(p - n + N_I^+\right) \tag{5}$$

with boundary conditions $\psi(\mathcal{B})$ depending upon the external voltages.

In our approach [3] the Poisson equation is not solved directly. $\psi(\mathbf{r})$ is separated to four components:

$$\psi(\mathbf{r}) = \psi_n(\mathbf{r}) + \psi_p(\mathbf{r}) + \psi_i(\mathbf{r}) + \psi_{\mathcal{B}}(\mathbf{r}) \tag{6}$$

where the first three components are simply calculated by using the Coulomb law

$$\psi_k(\mathbf{r}) = -\frac{q}{4\pi\varepsilon} \sum_j \frac{1}{|\mathbf{r} - \mathbf{r}_j|} \qquad k = n, p, I \tag{7}$$

The fourth component is given by the solution of the Laplace equation

$$\text{div grad } \psi_B = 0 \tag{8}$$

with a modified boundary condition, obtained by subtracting the potential values at the boundary $\mathcal{B}$ given by the electrons, holes and ionized impurities, ie.

$$\psi'(\mathcal{B}) = \psi(\mathcal{B}) - (\psi_n(\mathcal{B}) + \psi_p(\mathcal{B}) + \psi_i(\mathcal{B})) \tag{9}$$

This last step requires of course the numerical solution of the differential equation.

TIMING CONSIDERATIONS

One of the most crucial question of the Monte Carlo simulation is the choosing of the right *time step*. Several aspects about this issue are trivial. To follow the carrier motion properly, the elementary time step should be less than the average time interval between scatterings. Other factors influencing the allowable time step of the simulation are the followings:

- Errors having *numerical* origin. For example, the error arising from the linearized solution of the differential equation of the classical laws of motion.
- Errors having *physical* origin. The Heisenberg relation gives a restriction for the accuracy of the determination of the space and momentum coordinates.

The detailed analysis [4] shows that *linearization errors* of the space coordinates and momentum depend linearly on the ionized impurity concentration N_i, on the field E and on the average scattering time t_{scat}. This analysis results in an upper limit for the elementary flight time Δt.

$$\delta\mathbf{r} = L_0 \frac{N_I}{n_i} \frac{q\,E\,\tau_{scat}}{P_{max}} \left(\frac{1}{3}\frac{n_{inv}}{N_I} + \left(1 - \frac{n_{inv}}{N_I}\right)\frac{\Delta t}{\tau_0} \right) \left(\frac{\Delta t}{\tau_0}\right)^3 \tag{10}$$

$$\delta\mathbf{p} = P_0 \frac{N_I}{n_i} \frac{q\,E\,\tau_{scat}}{P_{max}} \left(\frac{1}{2}\frac{n_{inv}}{N_I} + \left(1 - \frac{n_{inv}}{N_I}\right)\frac{\Delta t}{\tau_0} \right) \left(\frac{\Delta t}{\tau_0}\right)^2 \tag{11}$$

The Heisenberg principle gives a relation between the uncertainty of the space coordinate dr and the uncertainty of the momentum dp as

$$\delta\mathbf{r} \,.\, \delta\mathbf{p} \geq h \tag{12}$$

For a particle having a space coordinate **r** and a momentum **p** at a time instant t, these quantities change to $\mathbf{r} + \Delta\mathbf{r}$ and $\mathbf{p}+\Delta\mathbf{p}$ after a small Δt. Let the uncertainties caused by the Heisenberg principle be

$$\delta\mathbf{r} = \alpha_r \Delta\mathbf{r} \quad \text{and} \quad \delta\mathbf{p} = \alpha_p \Delta\mathbf{p} \tag{13}$$

Substituting the space coordinate and momentum changes yields

$$\alpha_r \, \alpha_p \;\; m^{-1} \cdot \left(\mathbf{p}(\mathbf{r}(t),\; t) \;+ \frac{1}{2} \mathbf{F}(\mathbf{r}(t),\; t) \cdot \Delta t \right) \mathbf{F}(\mathbf{r}(t),\; t).\; \Delta t^2 \geq h \qquad (14)$$

Based on this equation, the lower limit for Δt at high fields is given by [5]

$$\Delta t = \tau_0 \left(\frac{|\mathbf{E}|}{E_0} \right)^{-2/3} \frac{1}{\alpha^{2/3}} \qquad (15)$$

NOTATION

quantum mechanical time unit $\tau_0 = \dfrac{h}{kT} = 1.600 \cdot 10^{-13}$ [s]

thermal (de Broglie) wave length $\lambda_0 = \dfrac{h}{\sqrt{2 m_0 k T}} = 7.623 \cdot 10^{-9}$ [m]

characteristic field $E_0 = \dfrac{U_T}{\lambda_0} = 3.389 \cdot 10^{6}$ [V/m]

intrinsic Debye length in silicon $L_{Di}^2 = \dfrac{\varepsilon_{Si} k\, T}{2 q^2 n_i} = 2.671 \cdot 10^{-5}$ [m]

characteristic length of carriers $L_0 = \dfrac{\lambda_o^4}{L_{Di}^2 a} = 8.736.10^{-15}$ [m]

characteristic momentum $P_0 = 2 \dfrac{m_0 L_0}{\tau_0} = 9.949.10^{-32}$ [VAs^2/m]

max. momentum (1. Brillouin zone) $P_{Max} = \dfrac{h}{a} = 1.220 \cdot 10^{-24}$ [VAs^2/m]

characteristic time $\tau_1 = \tau_0 \left(\dfrac{P_0}{P_{Max}} \right)^{1/2} = 3.018 \cdot 10^{-14}$ [s]

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