NUMERIC SIMULATION OF NONLINEAR DIFFUSION

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ABSTRACT

This article describes the development of a one dimensional simulator for nonlinear diffusion of dopant atoms in a semi-conductor. Based on the differential equations for linear and nonlinear diffusion a simulation model was elaborated and using the finite differences method this model was implemented with C++ into a simulation software.

1 INTRODUCTION

Surface diffusion is one of the most important physical principles the integrated circuit technology is based on. Dopant atoms are deposed on a semi-conducting base material at specific positions in order to alter the electrical properties. During the doping process, diffusion of the deposed dopant atoms into the base material occurs.

In fact of the steady evolution of integration technologies it is necessary to simulate more often in order to avoid high prototype costs and to simulate better in order to get process parameters with the needed accuracy.

2 SIMULATION MODEL

In currently used integration technologies, the regions where dopant atoms are implanted can become so small that a simple model of linear diffusion is not accurate enough. More accurate is the model of nonlinear diffusion, also called “extrinsic diffusion”: During a diffusion process, dopant atoms have a smaller mobility in the base material than their electrons (or holes). Thus, the electrons are tending to diffuse forward in the material leaving ionized dopant atoms behind. An electric field between the electrons and the ions will appear which will help the dopant atoms to diffuse faster inside the base material. This can be modeled by an additional flux in the classic diffusion law [1]:

$$F_{\text{total}} = F + F' = -D \cdot \frac{\partial C}{\partial x} + C \cdot v \tag{1}$$

($F, F' \ldots$ material flux, $C \ldots$ dopant concentration, $D \ldots$ diff. const. and $v \ldots$ drift velocity).

Considering the simplifying assumptions that all dopant atoms are ionized and that the investigated region has no total charge, the additional flux can be integrated into the differential equation for diffusion (Fick's 2nd law) by transforming it into the so called "field-enhancement factor" ξ:

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left[\xi(C) \cdot D \cdot \frac{\partial C}{\partial x}\right] \quad \text{with} \quad \xi(C) \equiv 1 + \frac{C}{\sqrt{C^2 + 4n_i^2}} \tag{2}$$

3 FINITE DIFFERENCES METHOD (FDM)

In order to simulate nonlinear diffusion according to the differential equation (2), it is necessary to transform it into a discrete form. This is necessary, because there is no analytic solution for this type of differential equation. A discrete form can be found by using the finite differences method (FDM).

For this method a discrete notion of time and space is necessary: the simulated material (total length L) is dissected into m samples and the time (total duration T) is split into n samples: $h = \Delta x = \frac{L}{m}$ and $k = \Delta t = \frac{T}{n}$. This one dimensional space can be represented as a two dimensional grid where every point at the location x_i and time t_j has an associated value of dopant concentration $u_{i,j}$. Now it is possible to replace each differential quotient by its corresponding difference quotient (first term of a polynomial Taylor approximation):

$$\frac{\partial C}{\partial t} \to \frac{\Delta u}{\Delta t} = \frac{u_{i,j+1} - u_{i,j}}{k} \quad \text{and} \quad \frac{\partial^2 C}{\partial x^2} \to \frac{\Delta(\Delta u)}{\Delta x \cdot \Delta x} = \frac{u_{i-1,j+1} - 2u_{i,j+1} + u_{i+1,j+1}}{h^2} \tag{3}$$

Using this, the differential equation (2) can be transformed into a discrete version:

$$\underbrace{u_{i,j}}_{\text{known conc.}} = \underbrace{\frac{-k \cdot D}{h^2}}_{const:\kappa} \cdot \underbrace{\xi(u_{i,j+1})}_{\text{field-enh. factor}} \cdot \underbrace{\left(u_{i-1,j+1} - 2u_{i,j+1} + u_{i+1,j+1}\right) + u_{i,j+1}}_{\text{unknown concentrations at time step } t_{j+1}} \tag{4}$$

The unknown concentrations of all points at the time t_{j+1} can be determined from the known concentration at the time t_j. A solution for every time step t_j can be calculated starting from known concentrations at t_0 by solving equation (4) for all intermediary time steps and all points of each time step. In order to solve such an equation system, it is necessary to include a boundary condition at the corner points outside of the considered space ($u_{0,t+1}$ and $u_{m+1,t+1}$). The Neumann boundary conditions were used, because they define that there is no flux of atoms between the inside and the outside of the considered piece of material. This means $\frac{\Delta u}{\Delta x} = 0$ at both borders.

In the defined simulation model, the concentrations at the different points are in a nonlinear relation. Applying a direct solving method is not possible: an iterative solver must be used. A very common solving principle for nonlinear equation systems is the multidimensional Newton principle. It can be easily customized to meet specific boundary conditions.

Using the Newton method, the iterative approximation of the searched concentrations must be interrupted by a break condition when the desired precision is reached. Two types

of conditions are necessary: The precision is high enough when the roots of the equations are near enough to zero and it is useless to continue when the difference between two iteration steps becomes to small to be relevant. Considering both conditions at the same time minimizes the computation time.

4 IMPLEMENTATION

The goal was to implement a software that is able to simulate the classic linear and the advanced nonlinear diffusion model in a one dimensional space. The implementation was done in two steps: First, the mathematical model and the Newton solver were defined in Matlab in order to quickly test the elaborated model. Then an object oriented software design model was created which was finally coded in C++ (system-independent using GNU-gcc). Graphical output was generated using GNUPlot.

5 SIMULATION RESULTS

A diffusion process at the temperature of 1100 °C on a piece of 300 nm length was simulated. Typical parameter values were chosen and a Gaussian bell curve was used as the starting concentration profile. The result (Fig. 1) shows the concentration profiles along the x-axis for linear and nonlinear diffusion after two different diffusion durations. The difference between the linear and the nonlinear model is about 10% which justifies the better model for submicron processes.

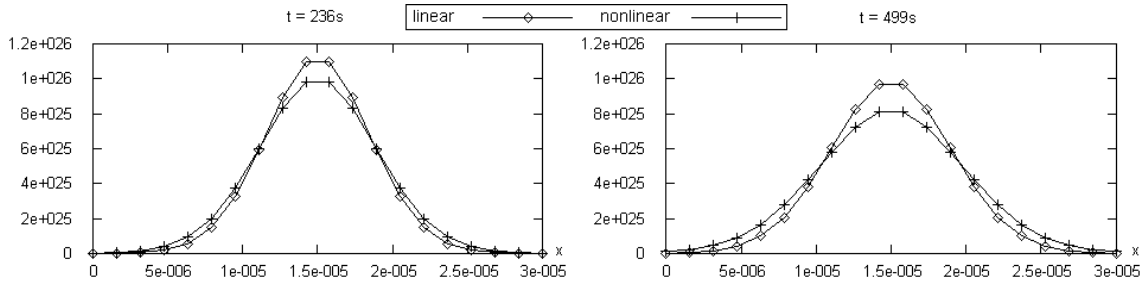

Figure 1: Linear vs. nonlinear diffusion (x: location [cm], $y = u$: concentration [cm^{-3}]).

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