SILICON INTEGRATED CIRCUIT FABRICATION PROCESS MODELLING AND SIMULATION

By

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1. Introduction

Nowadays, the up-to-date integrated circuits—all but a few cases—are made of silicon. There are two main phases of designing the circuits:

1. the design of surface structure (logical diagram[1], sub-circuits, layout, masks)

2. the design of vertical structure (perpendicular to the surface).

Early in the 1970's when SSI/MSI circuits prevailed, these phases could sharply be distinguished. The first design phase could still be divided into several independent design sub-phases, permitting a sharp distinction between the duties of the logical, circuit, and layout designer. These much differed from the scope of the semiconductor technologist designing the second phase.

By now the situation has fundamentally changed, for two main reasons:

1. Advent of new, higher circuit density devices (CCD, I^2L), which cannot be dissolved into separate components, they alone can stand for a whole (sometimes not even simple) logical function.

2. Better economy of achieving high density in LSI/VLSI circuits by decreasing stripe width than by increasing the surface (advantageous both for velocity and dissipation).

The smaller stripe width underlined the importance of the undesirable interaction between the surface, and vertical structure (e.g. lateral diffusion). On the other hand, this means that a good circuit can only be realized if the 1st and 2nd phases of planning are carried out by closely co-operating designers. With the increased complexity of integrated circuits the testability is becoming primordial in each stage of the design.

In the following the technological process simulating program *STEP* (*S*ilicon *T*echnology *E*valuation *P*rogram) now under development at the

[1] First of all digital circuits are meant, because in analog circuits: a. nowadays the main types have more or less been developed, b. they are seldom above SSI or MSI level, c. circuit technique tends to solve circuit functions increasingly by digital methods.

Department of Electronic Devices of the Technical University, Budapest, in co-operation with the Central Research Institute for Physics will be discussed. This paper is a short survey of problem of diffusion, while a further issue will be spent on ion implantation. The main point is the problem of oxidation.

2. Input and output data

The parameters of the main steps of silicon integrated circuit technology serve as input data of the program:

1. Predeposition
2. Drive-in
3. Epitaxial growth
4. Oxidation
5. Ion implantation
6. Etching
7. Oxide/Nitride deposition
8. Metallization/Polysilicon deposition.

Steps 1—4 are carried out at a temperature where, owing to the diffusion of dopants, their distribution changes. The steps 5—8 usually require a low temperature where the impurity distribution in the silicon remains unchanged. The user oriented input language is quite similar to the input format of the program SUPREM II of Stanford University Integrated Circuit Laboratory, published in June 1978. [1]. After the simulation of each technological step, all dopant distributions are available, from which, according to the user's demand, the postprocessor segment of the program can display:

a) graphically the distribution of dopants or of the resultant concentration of the electrically active dopants,

b) vertical dimensions (oxide) nitride thicknesses, junction depths,

c) electronic parameters of the semiconductor layers (sheet resistance, transport factor, punch through voltage),

d) the electronic parameters of the junctions (low-level $I-U$ characteristics, emitter efficiency, space charge capacitance, breakdown voltage),

e) MIS structure characteristics (oxide/nitride capacitances, MOS capacitance, threshold voltage).

3. Algorithm and model of diffusion

The behaviour of the dopants inside the material is described by the continuity equations

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{(V)} C_i \mathrm{d}V = \int_{(V)} G_i \mathrm{d}V - \int_{(S)} J_i \mathrm{d}S \tag{1}$$

set up for each dopant and the transport equations (I. Fick's law)

$$J_i = -\text{grad}\,(D_i \cdot C_i) \tag{2}$$

where C_i the i-th impurity concentration,
G_i generation rate per unit volume during unit time of the electrically active i-th impurity concentration (e.g. interstitial → substitutional transition),
J_i the i-th impurity flux,
D_i the i-th impurity diffusion coefficient.

According to the theory of diffusion the migration of dopants and the interaction of dopant species is taken into consideration so as they occupy different charge states of vacancies, (neutral, positive, singly or doubly negative) that is, the diffusion coefficient:

$$D = D^0 + D^+ V^+ + D^- V^- + D^= V^= \tag{3}$$

where the relative concentration of vacancies (referred to the intrinsic electron concentration) is:

$$V^+ = \frac{n_i}{n}; \quad V^- = \frac{n}{n_i}; \quad V^= = \left(\frac{n}{n_i}\right)^2 \tag{4}$$

In each point the n value is determined by the resultant electrically active dopant concentration. This theoretical method gives results deviating by orders of magnitude from those obtained by the simple phenomenal one—in good accordance with empirical results. In the continuity equation (1) J_i means exclusively the dopant flux according to Eq. (2) and G_i, with a few exceptions, can be neglected in the model of diffusion processes. Some algorithmic problems arouse at the $Si-SiO_2$ interface, due to

- the different diffusion coefficients of the layers and
- the flux at the interface

$$J_s = h\left(C_{0x} - \frac{C_{Si}}{S_{12}}\right) \tag{5}$$

where h is the surface mass-transfer coefficient,
S_{12} the equilibrium segregation coefficient,
C_{0x}, C_{Si} are concentrations at the interface.

The practically common diffusion anomalies, due to phosphorus overdosage will be taken with the model suggested by *Fair* and *Tsai* into consideration [2]. In lack of a well-founded theoretical model—an empirical

correction will be applied to modify the change of diffusion coefficient—in the presence of dry or wet oxigen. For details of the diffusion model and the solution algorithm let us refer to [3].

4. The model and algorithm of oxidation

The algorithm problem caused by the motion of silicon – silicon dioxide interface during the oxidation is more complicated than that of the diffusion processes. The dopant transport induced by the moving boundary can be described (for each dopant separately) by a dopant flux:

$$J_f = -V_{0x}(C_{0x} - \alpha C_{\mathrm{Si}}) \tag{6}$$

This equation simply expresses how much impurity gets absorbed with the oxidizing silicon by the oxide while the oxide thickness is growing at a rate v_{0x}. The α value of 0.44 means that 0.44 volume units of silicon produce 1 volume unit of silicon dioxide. The rate of oxide growth will be expressed by the equation suggested in [1].

$$Z_{0x}^2 + A \cdot Z_{0x} = B \cdot (t + \tau) \tag{7}$$

$$Z_{0x} = \frac{1}{2}\left[-(2 \cdot Z_{0x} + A) + \sqrt{(2 \cdot Z_{0x} + A)^2 + 4B\Delta t}\right] \tag{8}$$

in incremental form.

In these expressions the factors A and B are proportional to the partial pressure of oxygen and depend exponentially on temperature according to Arrhenius' law.

The investigation of this model has shown that the quadratically growing time step, found to be very good for the convergence of the solution of diffusion processes, can be used for the oxidation as well.

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Summary

The paper shows a computer based method, developed at the Department of Electronic Devices, Technical University, Budapest, for modelling the steps of the up-to-date silicon integrated circuit planar technology:

a) diffusion,
b) ion implantation,
c) oxidation,

d) chemical predeposition,
e) photolitography, etching.

Simulation helps predicting electrical parameters of the semiconductor structure (sheet resistances, current gains, MOS threshold voltage, etc.) during each of the technological steps. The simulation can involve all common donor or acceptor dopants (more impurity species as well) and the method also takes the interactions between the dopants into consideration.

The results obtained by simulation can be used as input data for a physical modelling computer program, for the optimum design, and subsequently, for the automation of technology.

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