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3D PROCESS MODELLING ON PERSONAL COMPUTERS

A. Zur, V. T. Binh

Technische Hochschule Ilmenau, DDR

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Abstract

A method for reducing the computation needs of modelling complete fabrication processes for VLSI devices on personal computers in 3 dimensions, a treatment of equations of basic physical processes, such as diffusion, oxidation, implantation, etching and deposition is presented. In the paper we will describe the structure of the TEDI (Technology Dialog) program, the main formulas and principles of the models and some examples of 3D process simulation. The third part of the 'TEDI' program (creating a set of control parameters, automatic simulation and graphical output of results) provides flexible possibilities of studying the connections between 1D, 2D and 3D simulations.

Keywords: Process modelling, VLSI technology

Introduction

The further reduction of the dimensions of IC-structures requires the modelling of technological processes in two and three dimensions. For instance, the calculated profiles and oxide layer thickness in small arrays, in corners are different in 1D, 2D and 3D simulations. On the other hand, the 3D device modelling, which is necessary to obtain the VLSI-device behaviour, gets its input data from 3D process models. In this work, we will discuss our 3D process model 'TEDI' (technology dialogue), which is capable of computing such complex processes as mentioned above in a simplified form on IBM XT/AT personal computer. The three-dimensional problems, of course, require much computing time, typically up to 8 hours. That is why one should perform identical 1D and 2D computations before a 3D one. The lower dimensions simulations can verify the correctness of simulation parameters, discretization of the structure and the influence of any special effects. Therefore, TEDI contains 1D and 2D models, too.

Program structure

The program 'TEDI' consists of 3 parts:
TEDPAR — a user interface dialogue for the automatic organization of the process simulation. The set of parameters begins with the definition of the format (1D, 2D, 3D) and the sizes of an actual cross-section. A set of parameters contains up to 20 process steps and includes reading or writing of external structure/concentration files. It is possible to correct or to change individual steps and parameters.
TEDAUT — automatic simulation and storage of results on the basis of a set of parameters. It contains a model controller and all numerical models of the process steps. This program is, therefore, designed to handle all formats (1D, 2D or 3D) in order to prove the correctness of input data for longtime 3D calculations by 1D calculations.
TEDRES — numerical or graphical output of results of process simulation. This program contains graphical algorithms for cross-section presentations with iso-lines, 1D-profiles, 2D-profiles and 3D-iso-lines. It can also produce output files for a device model interface.

Models

The exact solution of a 3D-implantation problem in complicated multilayer structures can be obtained using the Monte-Carlo-Models or by solving the Boltzmann-transport-equation. For PC-application we have used the first order approximation with Gaussian distributions (RUNGE, 1977) in the form of the following integral equation

$$N(x,y,z) = \int_{-\infty}^{+\infty}\int \frac{N_o(x',y',z')}{\sqrt{2\pi}\cdot\Delta R_x\cdot\Delta R_y\cdot\Delta R_p}\cdot$$

$$\cdot\exp\left[-\frac{(x'-x)^2}{2\Delta R_x}-\frac{(y'-y)^2}{2\Delta R_y}-\frac{(z'-z-R_p)^2}{2\Delta R_p}\right]\cdot dx\cdot dy \qquad (1)$$

with

x', y', z' — the point where a single ion passes through the target surface,
R_p — the projected range of ions,
$\Delta R_x, \Delta R_y, \Delta R_p$ — its standard deviation in each of the directions.

We calculate the parameters of these distributions for B, P, Sb, As in silicon on the basis of progressions given by (SELBERHERR, 1984). The algorithm can be used to predict 3D implanted profiles in multilayer structures with non-planar surfaces.

We may write the three-dimensional diffusion from a given initial distribution as

$$N(x,y,z,t) = \int \int\limits_{-\infty}^{+\infty} \int N(x',y',z'0) \times$$

$$\exp\left[\frac{-(x'-x)^2-(y'-y)^2-(z'-z)^2}{4Dt}\right] \cdot dx \cdot dy \cdot dz \qquad (2)$$

as it is shown by (LEE, DUTTON, 1981). This first-order approximation is assuming, in general, a concentration-independent diffusivity and the absence of other nonlinear effects, but by using a time step Δt in *Eq. (2)* instead of t it is possible to solve the nonlinear diffusion problem by integrating over Δt. Assuming only acceptors or donors as doping atoms, the diffusivity (HO, 1983) can be written as

$$D = \left(D^o + D^- \cdot \frac{n}{n_j} + D^+ \cdot \frac{p}{n_j} + D^= \cdot \frac{n^2}{n_j^2}\right) \cdot K_E \qquad (3)$$

with

$$K_E = 1 + \frac{1}{\sqrt{1+\frac{4n_j}{N}}},$$

— correction factor, based on the electric field in silicon,

$$n_j = n_i \cdot exp\left(\frac{\Delta E_g}{2kT}\right)$$

— stress-correction of the intrinsic density,

$$D^-, D^+, D^=$$

— diffusivity, caused by the vacancies.

The algorithm based on formulas (2) and (3) includes the computation of high-concentration distributions of phosphorus and arsenic, but does not include the interactions between boron and arsenic. Assuming an interfacial flux during oxidation and zero-diffusive-flux in SiO_2, equations (2) and (3) describe the evolution of impurity distributions during thermal oxidation. For 3D-simulation it is important that equations (1) and (2) contain similar exponential expressions, whose calculation will efficiently be supported by the coprocessor.

The algorithm of oxidation contains the well-known 1D-Deal-Grove-model, extended to a quasi-3D-model by stepwise calculation of the oxide thickness in all directions of interface movement. We obtain these directions with the graph-theoretical approach, which is described in connection with etching/deposition. The evolution of the volume of oxide results from a spherical wave model. This model assumes an increase in the SiO_2-volume by a factor of 2 and the expansion towards the nearest free surface. Thus it is possible to calculate such non-planar surfaces as they exist in all modern IC-technologies, and to obtain the moving boundaries for solving the redistribution problems. In the basic Deal-Grove-model we include all important effects like DEO (doping-enhanced-oxidation), thin-oxide correction, direction influence and wet/dry conditions. The advantage of this 3D algorithm is the short calculation time and the flexible assumption of arbitrary initial structures.

The etching and deposition processes are modelled in order to obtain initial structures for the main processes: implantation, diffusion, oxidation. Solutions providing higher accuracy require the use of special fine-line models. Our algorithm is based on a graph-theoretical approach for calculating a 3D-matrix which contains the minimum time required for etching each structure cell. The parameters for vertical and spatial etching/deposition define the type of the processes.

Examples

Fig. 1. shows 3D-iso-lines, obtained by two-step boron diffusion in silicon: $T = 1180°C$, $t = 240$ min. The iso-lines, as can be seen, describe a decrease in impurities under the mask edge and give a spherical profile in this region.

The implantation and diffusion of phosphorus in a very small window are also represented in *Fig. 2.*
These distributions correspond to an energy of 200 keV and dose of 10^{16} cm^{-2} and a single anneal step at a temperature of 1000°C and a time of 20 min. The parts 2 a), b) and c) show cross-section and phosphorus profiles, and the magnitude of redistribution during an anneal step.

Fig. 2. d) shows the comparison between 1D, 2D and 3D calculations of the same process. The great differences are due to a very small proportion of the size of the window to lateral standard deviation.

Finally, *Fig. 3.* shows a 3D oxidation step of a silicon trench with a Si_3N_4-oxidation mask.

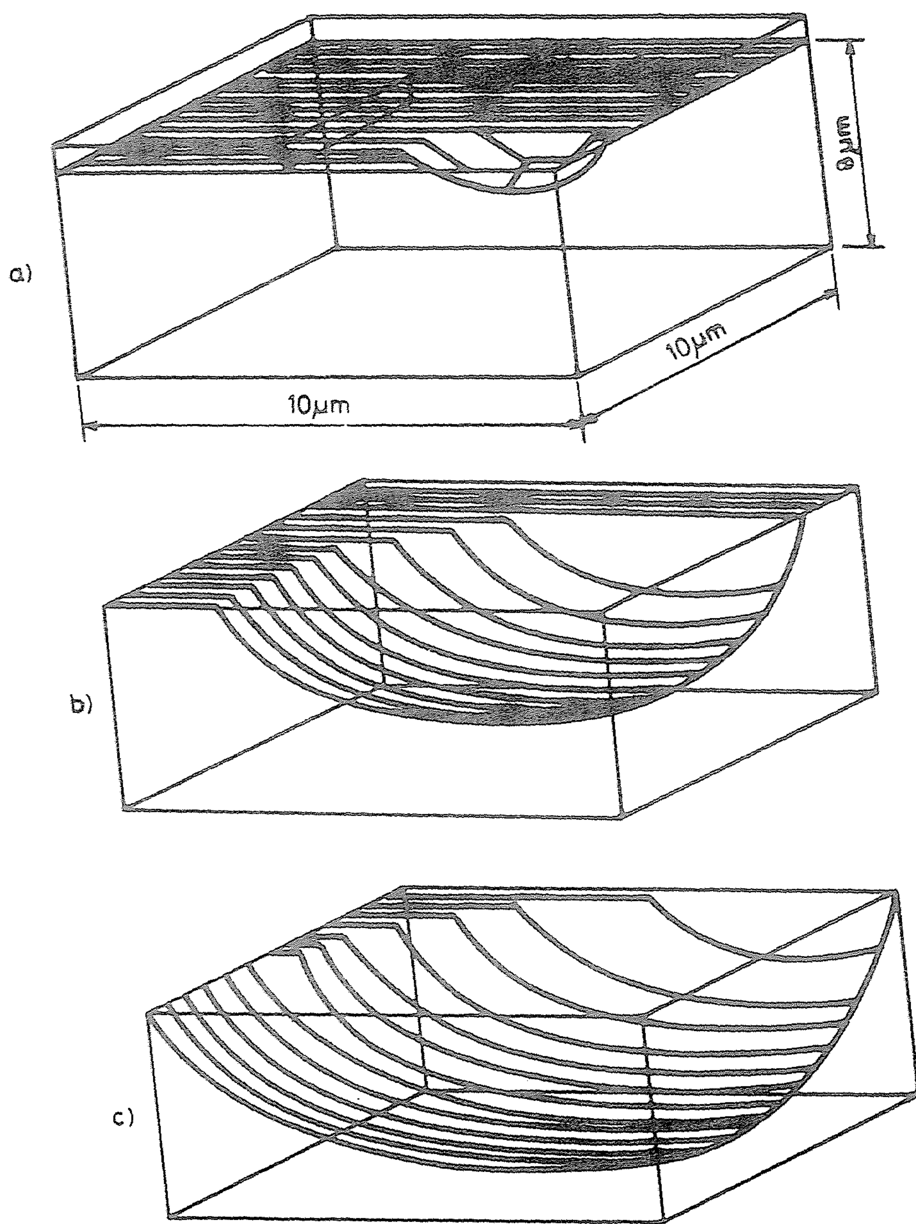

Fig. 1. Two-step diffusion of boron in silicon.
a) — $N = 10^{15}\,\mathrm{cm}^{-3}$, b) — $N = 10^{16}\ \mathrm{cm}^{-3}$, c) — $N = 10^{17}\ \mathrm{cm}^{-3}$

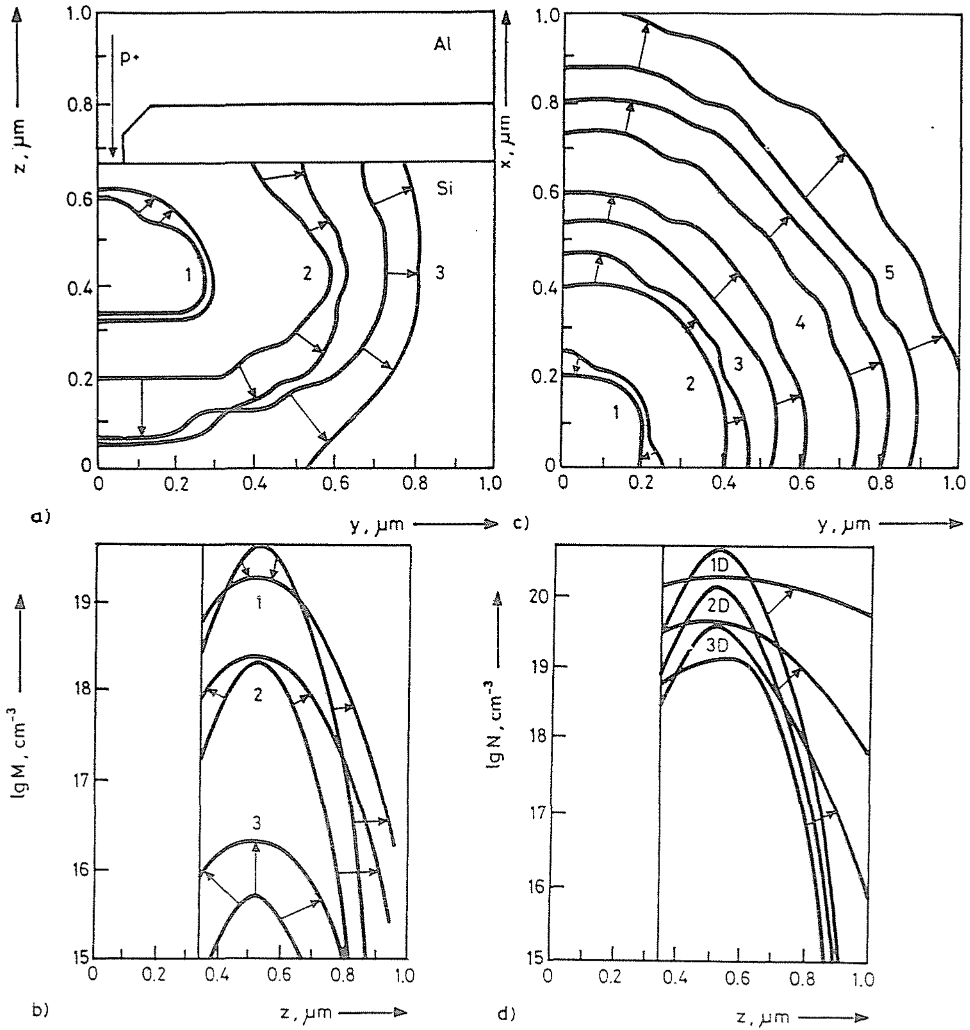

Fig. 2. 3D-implantation and diffusion of phosphorus
a) — $y - z$ cross section, 1 — $N = 10^{19}$ cm^{-3}, 2 — $N = 10^{17}$ cm^{-3}, 3 — $N = 10^{15}$ cm^{-3}
b) — phosphorus profiles, 1 — $x = .1\mu$m, $y = .1\mu$m, 2 — $x = .5\mu$m, $y = .5\mu$m, 3 — $x = .8\mu$m, $y = .8\mu$m.
c) — $x - y$ cross section. Curves 1–5 correspond to concentrations from 10^{19} to 10^{15} cm^{-3}
d) 1D, 2D, 3D comparison

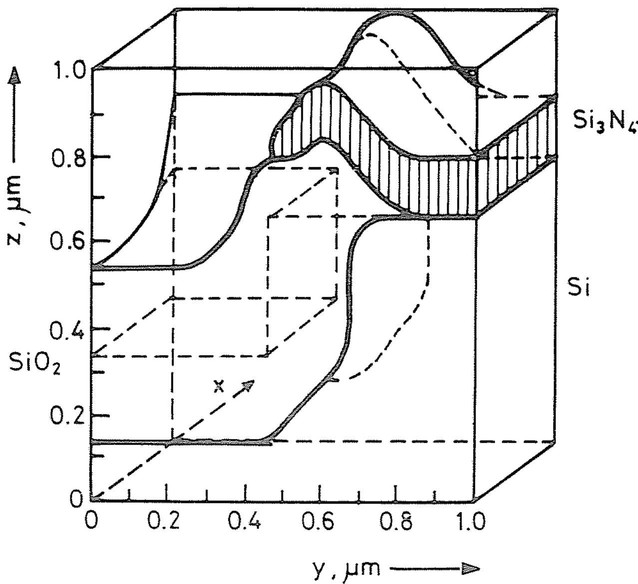

Fig. 3. 3D-wet-oxidation step of a silicon trench with a thickness of 0.4 μm.

5. Conclusion

The simplification of all basic models in VLSI-technology enables the simulation in 1–3 dimensions on personal computers. Such computations help to prepare simulations with higher accuracy, for example, on exact supercomputer models and to understand the influence of mask edges on profiles and oxide structures. We think that the TEDI model can effectively be applied both in the field of education and of computer-aided development of new VLSI-technologies.

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Address:

Prof. Dr. sc. techn. Albrecht ZUR
DI BINH Van Tran
Technische Hochschule Ilmenau
Am Ehrenberg
6325 Ilmenau
DDR