

(7A-1)

Extended performance of SUPREM4 for practical applications.

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Development of a process simulation program requires physical models, numerical mathematics and software engineering. Applicability to practical problems is not guaranteed, even if all three ingredients are present: A sophisticated program may lack just those features, that will make it a useful tool for the process engineer. We obtained the code of an early version of SUPREM4 from Stanford University (1) in order to apply it to problems in our laboratory. A number of alterations to the code and model parameters has adapted this program to some requirements for practical application. Examples from the process development in our laboratory and published applications of other process simulators provided us with a set of benchmarks for the applicability of the program.

Growth of field oxide was numerically simulated using the "viscous flow" model, but apparently no stiffness of the overlaying nitride mask was built into the original code, so that the nitride was lifted too much during oxide growth (fig.1a). The simulation in fig.1b shows a nitride layer resisting the oxide pressure; this result has been reached by giving the nitride viscosity coefficient an unphysically high value in the SUPREM4 input. This artificial resistance to bending gives the desired effect on the viscous flow of oxide. An experimental "suppressed" bird's beak resembles fig.1c; the oxide growth under the nitride is apparently reduced. While the cause of this reduction is still under discussion, this experimental fact could be simulated by dividing the silicon substrate in two regions, each with its own oxidation rate.

Oxidation of non-planar structures, like the mesa structure in fig.2 (2) is a more severe test to a process simulator. The expanding triangular mesh of SUPREM4 apparently gives a faithful simulation of the "crooked bird's beak".

Monocrystalline silicon was the only material for which oxidation could be simulated in the original program. Our applications (2), however, included structures like the one simulated in fig.3, where a polysilicon region borders the monocrystalline substrate and oxidation of both must be simulated. After some changes in the code had been made, nodes in polysilicon as well as in monocrystalline silicon could be transformed into oxide.

SEM photographs form the experimental information, with which the simulation of a structure is verified; SIMS measurements are the most accurate data for verification of the parameter values used in the simulation of a dopant distribution. A fit of the boron diffusion coefficients to a series of SIMS curves was made using SUPREM3 (3). Such fitted values can be used in a SUPREM4 simulation of the indiffusion of boron from polysilicon (fig.3). Adaptation of parameters will remain necessary, as long as the physical models in a simulator are not valid under all process conditions, that occur in practical applications.

- (1) We thank prof. Dutton (Stanford University) for his permission to use the SUPREM4 code (version 3.1) for research purposes.
- (2) J. van der Velden, R. Dekker, R. van Es, S. Jansen, M. Koolen, P.Kranen, H. Maas, A. Pruijboom, Proc. IEDM 1989 233-236
- (3) K.J. van Oostrum, J. van Dijk, C.J. Vriezema, P.C. Zalm
Paper submitted to SSDM (1990)

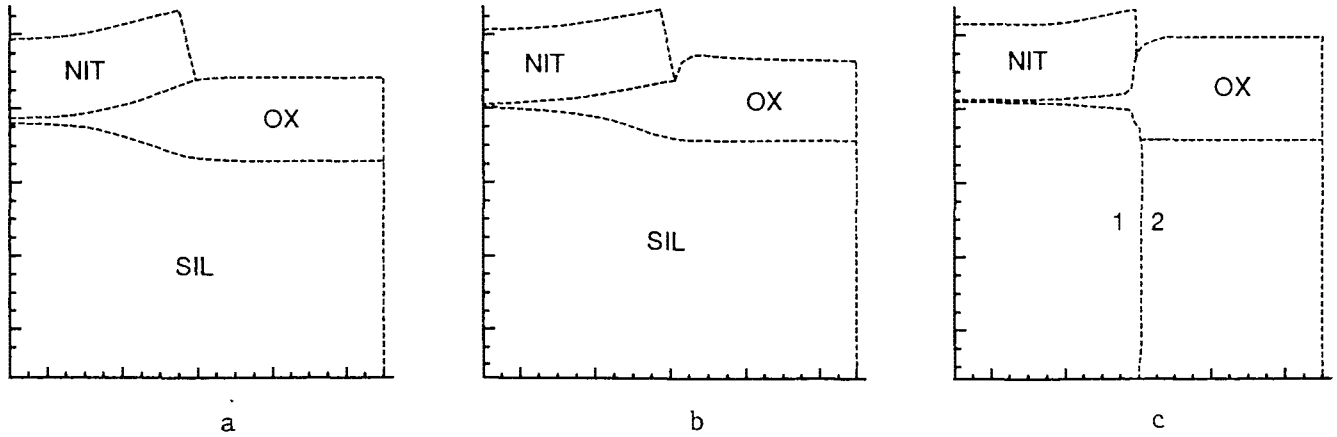


fig.1 Oxidation using the SUPREM4 viscous flow model with default parameters (a), high nitride viscosity coefficient (b), different oxidation rates in regions 1 and 2 of the substrate.

fig.2 SUPREM4 simulation of "crooked bird's beak" oxidation in BASIC mesa structure (2).

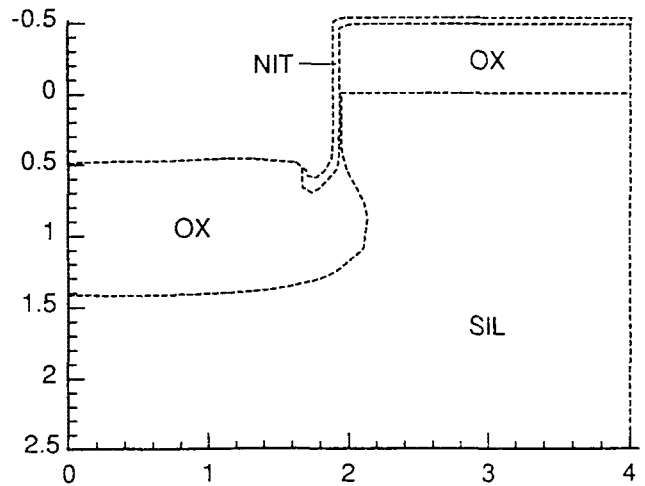


fig.3 Simulation of basis formation in BASIC (2) with oxidation of bordering polysilicon and silicon regions. Isoconcentration lines for boron: $1e15$ to $1e19$ cm^{-3}

