# QUANTITATIVE POINT DEFECT BASED 2-D PROCESS SIMULATIONS.

D. Collard (*) and K. Taniguchi

Toshiba Corporation, VLSI Research Center, Komukai Toshiba-cho, Kawasaki, 210 JAPAN.
(*) On leave from Institut Superieur d'Electronique du Nord (ISEN), 41 Boulevard Vauban, 59046 Lille Cedex, FRANCE.

Abstract

A point defect based process simulator IMPACT (**) have been developed. This program simulates both dopant and interstitial diffusion during the usual IC fabrication steps. A wide range of experimental results have been successfully simulated: 1D and 2D oxidation enhanced diffusion and diffusion enhancement due to backside oxidation. A complete set of model parameters for the interstitial redistribution is proposed.

## Introduction

To go on to be helpful in the development of the sub-micron technologies, the process simulators have to handle more accurate and reliable process models than nowadays. As the silicon point defects (interstitials and vacancies) are responsible for the dopants diffusion, a physical way to investigate new process simulations is to solve both impurity and point defects simultaneously. In a counterpart, performing this kind of simulation proved to be delicate as many new unknown parameters are added for the calculation of point defect redistributions.

This study focuses on the extraction of the interstitial model parameters by investigating the simulations of a wide range of experimental results in which interstitials are directly involved: 1D and 2D oxidation enhanced diffusion (OED) and diffusivity enhancement due to backside oxidations.

The resulted simulation program, IMPACT(**) [1], uses finite elements with strong local grid refinement.

## Process models

The interstitial redistribution is governed by the 2D diffusion equation, in which the bulk recombination with vacancies is assumed to be in thermal equilibrium. On the oxidized boundary, the interstitial flux is composed of, accordingly to Hu's model, a generation term, that is proportional to the local oxidation rate, Vox, and a surface recombination term:

$$D \cdot \mathrm{grad}\, C \cdot n = K \cdot Vox - h \cdot ( C - C^* ). \qquad \text{(eq. 1)}$$

C and D are the interstitial concentration and diffusion coefficient, respectively. The star (*) refers to the equilibrium value while h is the recombination rate.

The impurity diffusion equation is solved under its low concentration form with an effective diffusion coefficient, Deff, that is interstitial concentration dependant:

$$Deff = D^* \cdot \{ f\,(C/C^*) + (1- f)\,(C^* / C) \} \qquad \text{(eq. 2)}$$

## Model extraction

The surface recombination rate, h, was deduced from extensive simulations of lateral OED experiments [2], an activation energy of 1.8 eV, close to the Si-Si bound energy was found. Fig. 1 shows interstitial equi-concentration contours in the case of a LOCOS process (992 C, 69 hours) while Fig.2 presents a zoom in which the phosphorus doping profile is added. The lateral OED reduction under the non-oxidized area is obvious. Fig. 3 compares the measured and simulated OED reduction versus the nitride width. A good agreement is obtained for a wide range of processing conditions.

The proportionality factor K was optimized by matching an already proposed analytical expression of the excess interstitial concentration deduced from stacking faults measurements [3]. Contribution factor, f, is then extracted from many published OED data. Finally the overall model was successfully tested in the case of OED due to backside oxidation.

## Current work

The study of MOS narrow channel effect using this new model and the coupling with device simulator MOS2C [4] is still in progress, the first results will also be presented.

(**) ISEN Modeling PAckage for integrated Circuit Technology.

References
[1] D. Collard et al., To be published in IEEE-ED.
[2] K. Taniguchi et al., Appl. Phys. Lett., 43, p. 449, 1985.
[3] K. Taniguchi et al., Proc. Symp. on Defects in Silicon, p. 315, 1983.
[4] T. Wada et al., Proc. NASECODE 4 conf., p. 108, 1985.

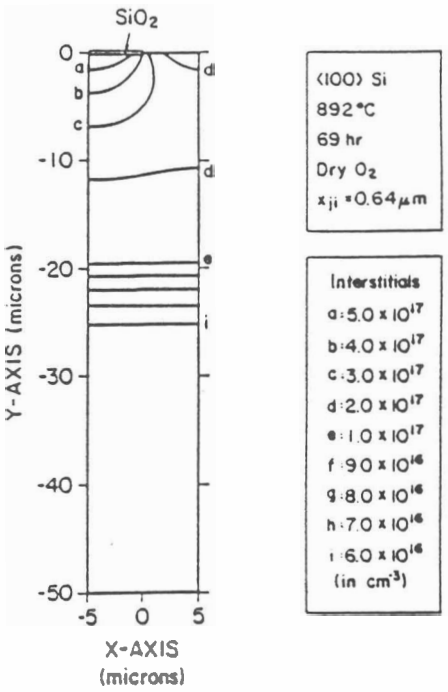


Fig.1 : Interstitial equiconcentration contours after a LOCOS formation.

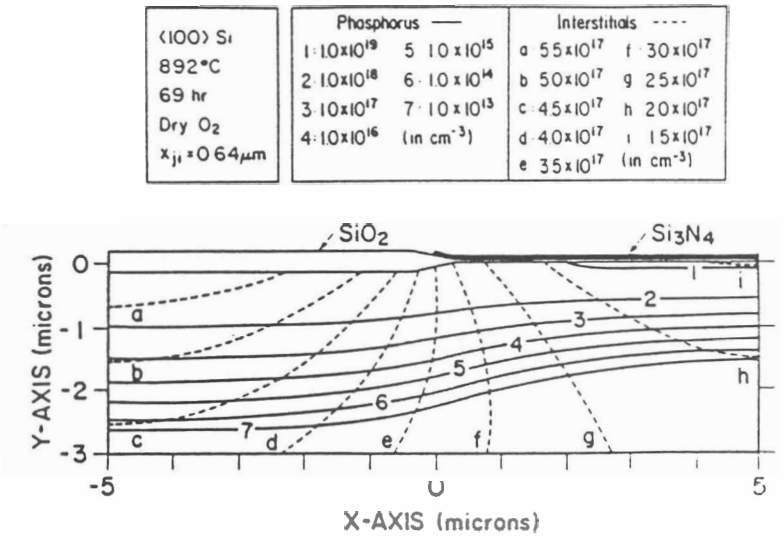


Fig.2 : Zoom of the upper part of Fig.1 with Phosphorus profile.

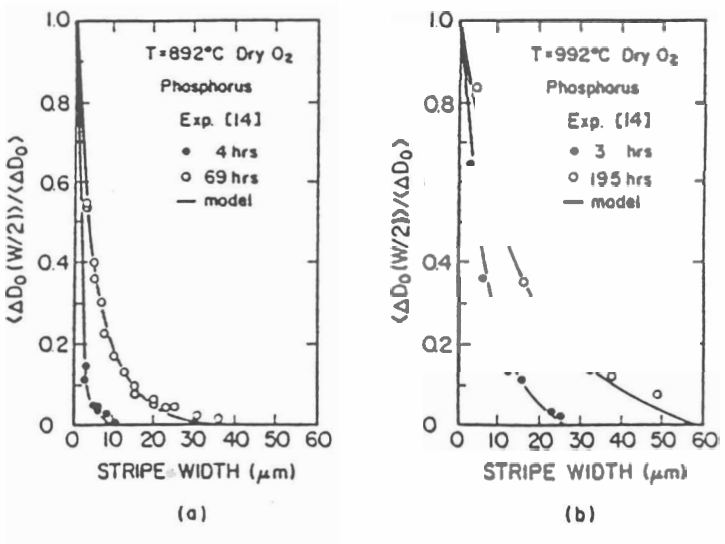


fig.3 : Lateral OED reduction vs. nitride stripe width. Comparison between experiments (point) and simulations (full line) for 2 temperatures: 892 C (a) and 992 C (b).