SIMULATION OF SEMICONDUCTOR DEVICES AND PROCESSES Vol. 4
Edited by W. Fichtner, D. Aemmer - Zurich (Switzerland) September 12-14, 1991 - Hartung-Gorre

Efficient Simulation of Impurity Segregation during Oxidation of Arbitrarily Shaped Multi-Layers Structures.

Dominique Collard, Bruno Baccus, and Emmanuel Dubois
ISEN, 41 Boulevard VAUBAN, 59046 LILLE Cedex, FRANCE.

Abstract

For the multi-layers process simulation, a large flexibility is needed in the mesh generation, specially to ensure a good convergence in stress dependent oxidation modeling. This paper presents an efficient numerical treatment for the solution of dopant redistribution and segregation when the mesh is completely re-generated at each oxidation step.

To be applied on up-to-date silicon technologies, the two-dimensional (2D) process simulators have to solve the impurity diffusion in all the present layers. Moreover, in order to ensure a good convergence in stress dependent oxidation modeling, a large flexibility is required for the oxide mesh generation. In this case , the moving boundary problem complicates the numerical treatment of dopant redistribution and segregation, specially in the cases of complex geometrical structures. An efficient numerical procedure has been proposed for 1D simulation [1], but its extension to 2D [2] requires a arduous numerical treatment and may lead to very large discretization point numbers. This paper proposes a new and simple method, based on the finite element method, that efficiently solves the impurity diffusion and segregation even in the case of arbitrarily designed meshes needed for stress effects analysis in oxidation simulation.

1 Numerical procedure

A triangular mesh is generated, using Delaunay criterion for the complete structure [3]. The same grid is used for the numerical oxidation simulation (oxidant diffusion and elasticity equations) and for the impurity diffusion. Fig. 1 shows a typical mesh used for this application.

For each oxidation incremental step, the following procedure is performed:

a) The interface and surface nodes motion is calculated from oxidant diffusion and elastic displacements.

b) The lost impurity quantity, Q_S, due to the interface motion is calculated for each oxidized layer (silicon and polysilicon). Q_S, depicted in fig.2(a), is calculated by an integration along the interface using the concentration and the concentration spatial derivatives in the oxidation direction given by the finite element shape function.

c) The interface are displaced and the total mesh is re-generated using the new interface nodes and a regular grid of internal points.

d) The impurity concentration are then interpolated in all the layers in anticipating the segregation phenomena. The silicon and polysilicon nodes concentrations are directly calculated from the previous structure. The new oxide nodes that belongs to the displaced old oxide layer are also interpolated on it. The static segregation is unforced on the the interfaces. A Laplacian is then solved on the oxide layer, the already interpolated nodal concentration being kept fixed, in order to estimate the concentration of the nodes belonging to the newly grown oxide, dT_{ox}. The scheme is illustrated in fig. 2 in which m is the segregation coefficient.

This interpolation scheme induced a impurity quantity increase, Q_I given by:

$$Q_I = Q_O - Q_S = Q_S \left(\frac{1}{\alpha m} - 1 \right) \qquad (1)$$

e) a diffusion step is then solved simultaneously for all the present layers. During this step, the interface boundary flux takes into account the static segregation and compensates the quantity Q_I in order to garanty the total dose conservation. The dose conservation flux term is distributed on the interface nodes with a ponderation proportional to the nodal $(V_{ox}.C)_i$ product, where V_{ox} and C are the oxidation rate and the concentration at the node "i". The flux condition at the interface node i is expressed by :

$$F_i = \frac{Q_I}{\Delta T} \frac{(V_{OX}\ C)_i}{\int_\Gamma V_{OX}\ C\ d\Gamma} \qquad (2)$$

where Γ is the oxidized interface.

2 Results

This new numerical technique is applied to the diffusion in wet ambient (1000° C, 2 hours) of a phosphorus doped (1.10^{17} at/cm3) substrate implanted with boron (100 KeV, 1.2 10^{12} at/cm^2). The computed doping profiles are compared with those obtained with SUPREM-II in fig.3. An excellent agreement is reached for both phosphorus and boron that exhibits opposite type interface segregation.

The application of the numerical technique to 2D exemple is illustrated in Fig. 4. A boron doped channel stopper diffuses during a polysilicon filled trench oxidation. The boron iso-concentration contours exhibits clearly the segregation mecanism at the Si/SiO_2 interface and an excellent numerical stability is reached, even for the profile in the grown oxide. The final mesh has been given in fig.1.

In fig.5 is dispayed the boron channel stopper profile in the case of a LOCOS field oxide. In this simulation, the stress effects have been intoduced in the oxidation kinetics accordingly to the model proposed by Kao [4]. This final result summarizes the major difficulties present in the coupling between oxidation and diffusion simulation.

3 Conclusion

A new numerical procedure for the simulation of dopant redistribution in multi-layers structures during oxidation has been developed. This procedure ensures a total dose conservation and has proved to be efficient even in the case of complex geometrical configuration.

Acknowledgements

The authors would like to thank Dr. A. Poncet from CNET/CNS for his fruitful advice.

References

[1] D.A. Antoniadis, M. Rodoni and R.W. Dutton, J; Electrochem. Soc. **126**, 1939 (1979).
[2] L. Borucki, H.H. Hansen and K. Varahramyam, IBM J. Res. Develop. **29**, 263 (1985).
[3] B. BACCUS et al., J. Solid States Electron., **32**, 1015 (1989)
[4] D.B. KAO et al., IEDM Tech. Dig.; 388 (1985)

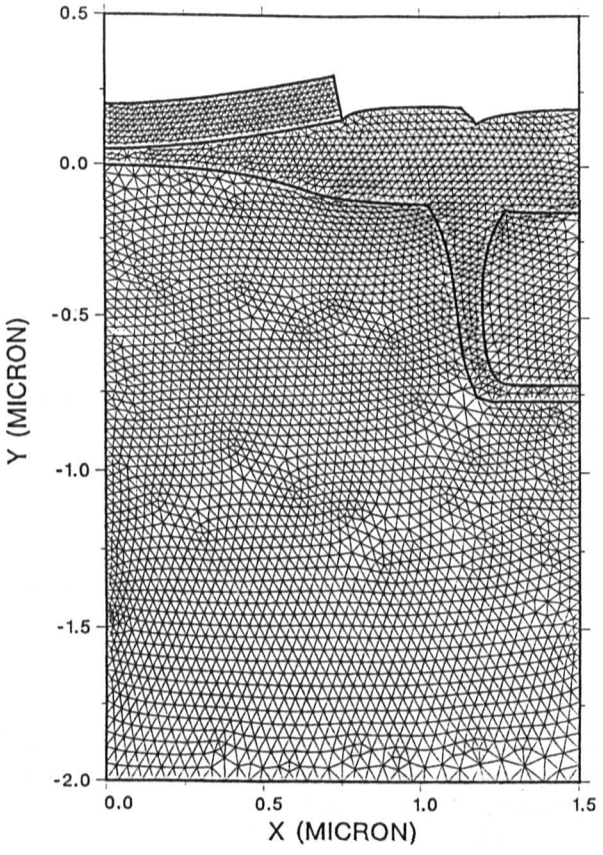

Figure 1: Finite element mesh for the multi-layers process simulation of a trench structure.

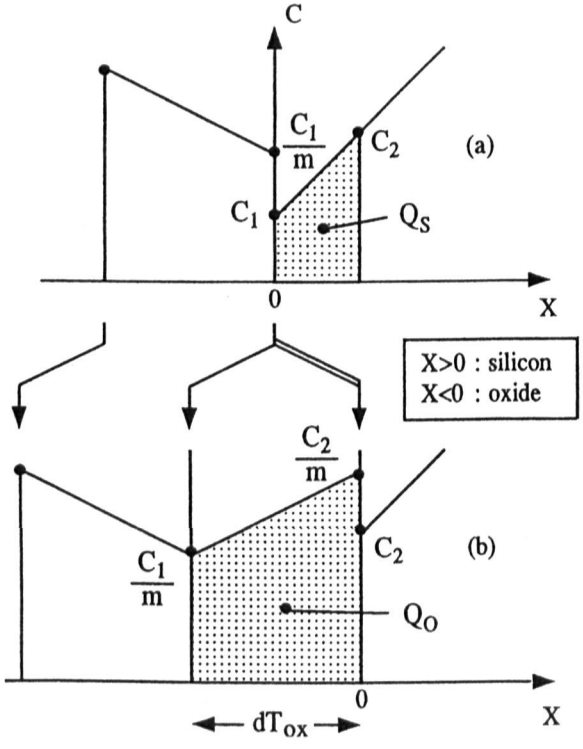

Figure 2: Concentration interpolation scheme for the moving Si/SiO_2 boundary. (a) Before the oxidation step. (b) After the Si/SiO_2 motion corresponding to an oxide growth thickness dT_{ox}.

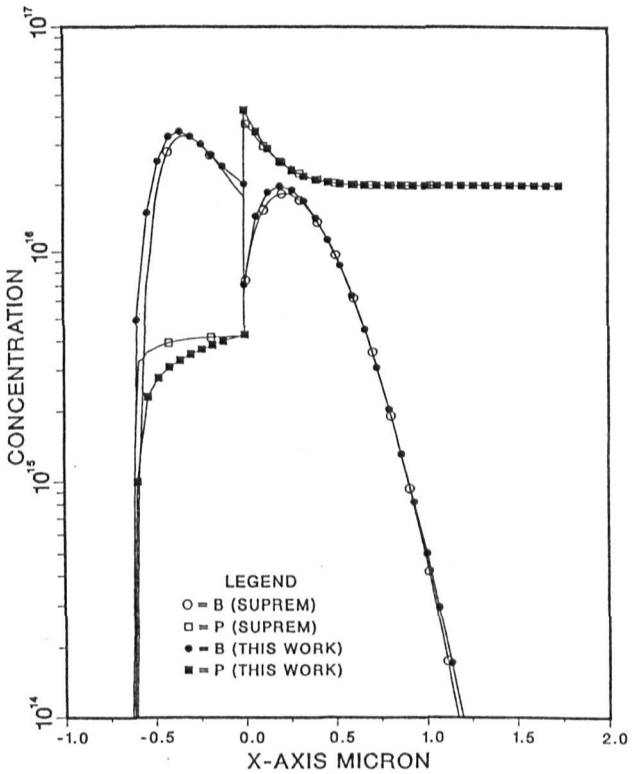

Figure 3: Simulated phosphorus and boron profiles after a wet oxidation, comparison with SUPREM-II results.

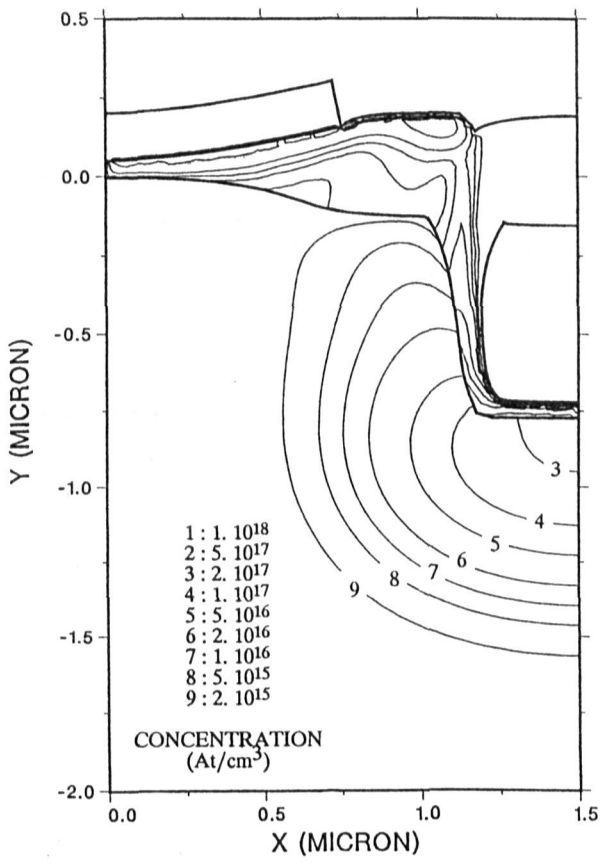

Figure 4: Boron iso-values contours in the structure of fig.1 after the trench oxidation.

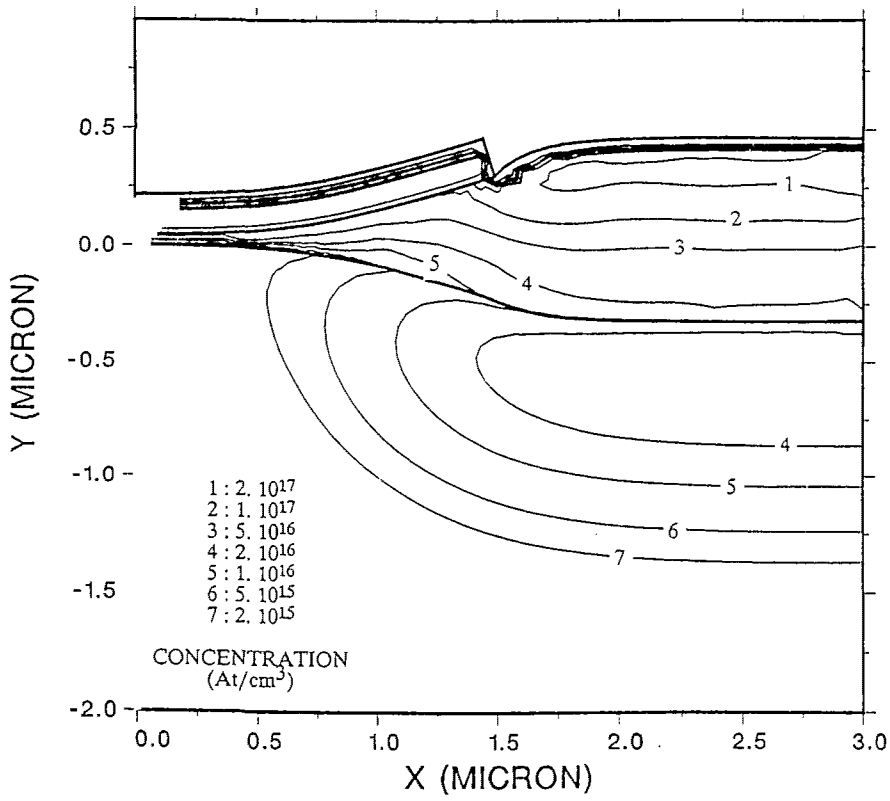

Figure 5: Boron concentration iso-values contours in a LOCOS structure. This simulation includes the stress effects in the oxidation kinetics.

.