COMPUTATION OF THE HYDRODYNAMICS OF 2D OXIDATION PROCESSES USING BOUNDARY FITTED COORDINATE SYSTEMS

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ABSTRACT

Simulation of semiconductor device is very difficult in 2 or 3 dimensional cases because of their irregular boundaries involved. Usually finite element method is prefered in these cases. But, despite of the flexibility to adapt to any geometry, this method doesn't have a whole approval of the scientific community because its programmation is long and tedious, except if a well documented subroutine library is available. Another method i.e. finite difference method is conceptually easier but requires a mapping from physical plane to rectangular coordinate plane. There are many procedures to generate this coordinate system. Among them, use of the Laplace equations, because of the simplicity of formulation and possibility of coordinate-line-spacing control, is very attractive.

Oxide here is considered as very viscous fluid floating upon a rigid silicon layer. System will contain besides Navier-Stokes equations and oxygen diffusion equation, two elliptic equations (actually their inverses are used). The first two groups of equations (which we refer as phisical) determine boundary of oxide domain which will be injected to the inverse elliptic equations (which we refer as transformation) to fix boundary conditions of the latters. Since physical equations require the transformation equations to be formulated, we have a system of completely coupled 6 equations. Increase of the number of equations is counterbalanced by the fact that we have now a partial differential equation system specified in fixed rectangular plane, so it is very easy to formulate in terms of the finite difference. Moreover there is no need for additional interpolation due to movement of the physical domain, because this is geniously incorporated in the above system.

1. INTRODUCTION

Oxidation is one of the most crucial parts of the semiconductor device fabrication processes besides impurity diffusion. Surprisingly, its numerical studies are rather scarce,

compared to the proliferation of the latters', partly because of the complexity of the numerical treatments. Recently Chin studied creeping flow of the oxide layer, using boundary value technique [5], which avoids finite difference or finite element formulation, more frequently used in physical simulations.

If you want to do a true 2 dimensional simulation of oxidation process with finite difference method, because of the complex geometry, some arrangments are necessary.

Actually, there are two different approaches for use in complex geometry.

a) Using a rectangle which embodies the whole physical domain of interests. Classical rectangular lattice is used so the finite difference formulation is straight way, but node points out of the physical domain is wasted and boundary condition is painfully handled.

b) Transformation of rectangular coordinate such a manner that it fits to the physical domain. All node points are meaningful and boundary treatments are more elegant. But physical equations become more complicated, and frequently number of equations increses.

We have chosen approach b) in this work but approach a) is also feasible. For exemple, MAC code [7] is one of the most popular and well tested programmes in fluid dynamics research, and it uses the latter approach.

2. TRANSFORMATION EQUATIONS

There are thousands of different methods [3] to generate coordinates fitted to the physical domain. We have chosen Thompsons' algorithm [1][2] because it can fit to any virtually all connex compact domains, with possibility of local coordinate refinements (this technique is not exploited in this paper).

We briefly summarize here his algorithm for the readers who are unfamiliar with it.

Consider a couple of elliptic equations defined in a physical plane (x,y) :

$$(1) \qquad \xi_{xx}+\xi_{yy}=0$$

$$\eta_{xx}+\eta_{yy}=0$$

If couple of variables (ξ,η) is the coordinate of a rectangular plane, this system forms a mapping of physical plane (x,y) to rectangular plane (ξ,η). Suppose that the boundary of a given compact physical domain corresponds to the frame of a rectangle and we have means of knowing the position of the physical boundary, then the resolution of the inverse system (2) becomes a typical Dirichlet problem.

$$(2) \qquad \alpha x_{\xi\xi}-2\beta x_{\xi\eta}+\gamma x_{\eta\eta}=0$$

$$\alpha y_{\xi\xi}-2\beta y_{\xi\eta}+\gamma y_{\eta\eta}=0$$

$$\text{with} \quad \alpha = x_\eta^2 + y_\eta^2$$

$$\beta = x_\xi x_\eta + y_\xi y_\eta$$

$$\gamma = x_\xi^2 + y_\xi^2$$

Its resolution gives us a correspondence between interior points of the physical domain and of the rectangle, so we can explain any physical equation in function of the rectangular coordinate system (ξ, η)

Subsequently, in order to simplify the presentation, we write all physical equations in (x,y) *plane but do not forget to transform them in* (ξ, η) *plane expression for the numerical treatments. For exemple*

$$f_x = \frac{\partial(f,y)}{\partial(\xi,\eta)} \Big/ \frac{\partial(x,y)}{\partial(\xi,\eta)} = \frac{y_\eta f_\xi - y_\xi f_\eta}{J}$$

$$f_y = \frac{\partial(x,f)}{\partial(\xi,\eta)} \Big/ \frac{\partial(x,y)}{\partial(\xi,\eta)} = \frac{-x_\eta f_\xi + x_\xi f_\eta}{J}$$

where J *is the Jacobian* $J = x_\xi y_\eta - x_\eta y_\xi$.

3. PHYSICAL EQUATIONS

3.1 bulk region

According to the Chin's idea [4], we suppose oxide layer forms a incompressible Newtonian fluid. Because the Reynolds number is very low in this case, the convective terms can be neglected before viscous ones, and Navier Stokes equations take the following form.

$$(3) \qquad u_x + v_y = 0$$

$$u_t = -\Phi_x + \nu \Delta u$$

$$v_t = -\Phi_y + \nu \Delta v$$

where (u,v) *is velocity in* (x,y) *plane*
$\Phi = p/\rho$ *is normalized pressure with* ρ *oxide density*
$\nu = \mu/\rho$ *is kinematic viscosity with* μ *dynamic viscosity*

In order to avoid numerical difficulties due to the presence of the continuity equation i.e. we don't know any no trivial initial velocity distribution, and to make pressure value more tractable, we transform system (3) to the following form [7] by deriving the second equation by x and the third equation by y, adding them all together and simplifying with the help of the first equation but retaining the time derivative term D_t.

$$(4) \qquad \Delta\Phi = -D_t + \epsilon \Phi_t$$

$$u_t = -\Phi_x + \nu\Delta u$$

$$v_t = -\Phi_y + \nu\Delta v$$

$$\text{with } D = u_x + v_y$$

The time derivative of pressure is added as numerical artifice. ϵ positive quantity is fixed in function of precision required. It is smaller when more accuracy is desired.

The time derivative term retained D_t appears as source term of diffusion type equation and calculated as:

$$D_t = \frac{D(t+\delta t) - D(t)}{\delta t} = -\frac{D(t)}{\delta t}$$

It permits to relax any arbitrary initial velocity distribution to values satisfying the continuity equation [8].

We used here so called primitive variables (u, v, p) formulation. Fluid researchers should be also familiar with vorticity-stream function (ω, Ψ) formulation which uses only 2 variables instead of 3, but it has additional difficulties in boundary treatments, in particular in oxide-air interface where pressure value enters explicitly in boundary condition expression.

We have no comments about oxygen diffusion. We simply used the 2 dimensional parabolic equation with constant diffusivity

$$(5)\quad \frac{\delta N}{\delta t} = C\Delta N$$

3.2 *boundary conditions*

Boundary conditions used by Chin [5] is correct, except the free boundary i.e. oxide-air interface, condition. He has to use the normal and tangential stresses null condition, instead of the pressure equilibrium condition [6]. This is particulary true in high viscosity case.

In order to resolve analytically the system b), it is unnecessary to have overall boundary condition for all 3 primitive variables because this has the mixture of 1 and 2 orders space derivative terms. But for numerical treatments, this statement is false. Supplementary boundary conditions are necessary, otherwise the system would be singular. Troubles caused by introduction of the extra boundary conditions are well known by fluid reserachers [9] . They have to satisfy stability and accuracy conditions besides von Neumann condition applicable in bulk region [10]. Unfortunately overall accepatble procedure is not yet available. We used interpolation based formula because this is easy to apply, and accuracies and stabilities are not so bad [11].

3.3 *initial conditions*

Strictly speaking, simulation must begin with a zero thickness oxide pad. Naturally this is numerically unrealizable.

You have to choose some small thickness, but not too much small to avoid numerical difficulties. Oxygen density is nearly zero at silicon-oxide interface and there is no movement inside the oxide pad. Pressure is 1 bar everywhere.

4. PROGRAMMING

We have now a system of 6 partial differential equations defined in fixed and rectangular 2 dimensional domain (ξ, η) i.e.

Oxygen diffusion equation (5)
Navier-Stokes equations (3)
Quasi elliptic equations for coordinate change (2)

To be more accurate and perhaps to be more stable, we have to integrate simultanously 6 equations. In order to avoid to have a too big matrix to invert (in fact inversion cost is $O(n^2)$ in n dimensional banded matrix case), we treat this system of partial differential equations by 3 resolution steps. Firstly we resolve the diffusion equation and this gives us an oxygen concentration at silicon-oxide interface. This concentration is used for calculating boundary condition at silicon-oxide interface for Navier Stokes equations. So at second step we resolve 3 fluid equations. Velocity distribution so calculated is used for updating position of the physical boundary. Last step is the resolution of the quasi elliptic equations with the help of the boundary condition obtained at the second step. We can repeat this sequence until sufficient amounts of time elapse. Each linear system is resolved with one of the iterative methods proposed in [12].

5. RESULTS AND CONCLUSION

Because routine which calculates nitride deformation is not yet incorporated in our programme, we can tested only the case where thickness of the latter is infinite. So no-slip wall condition is applicated at nitride-oxide interface. Figure 1 represents geometry of the oxide layer after about 3 hours of oxidation. Despite coarse grids (total grid points 40 X 20, oxide-air interface 20 points, oxide-nitride interface 20 points), coordinate fitting algorithm works perfectly. A turn of silicon-oxide interface just under the end of nitride is visible. It corresponds to high gradient of oxygen concentration (fig. 2). Because this zone correspons to fast changes of physical parameters, the local coordinate refinement is desirable. It consists in adding source terms to elliptic equation system (1) [1]. Our future code will include this effect to obtain more accuracies and stabilities.

It takes about 2 hours of CPU time with DPS 8/70 processor to obtain this result.

We concluded that the finite difference method using Thompson's algorithm can well compete with the finite element method in complex geometry applications.

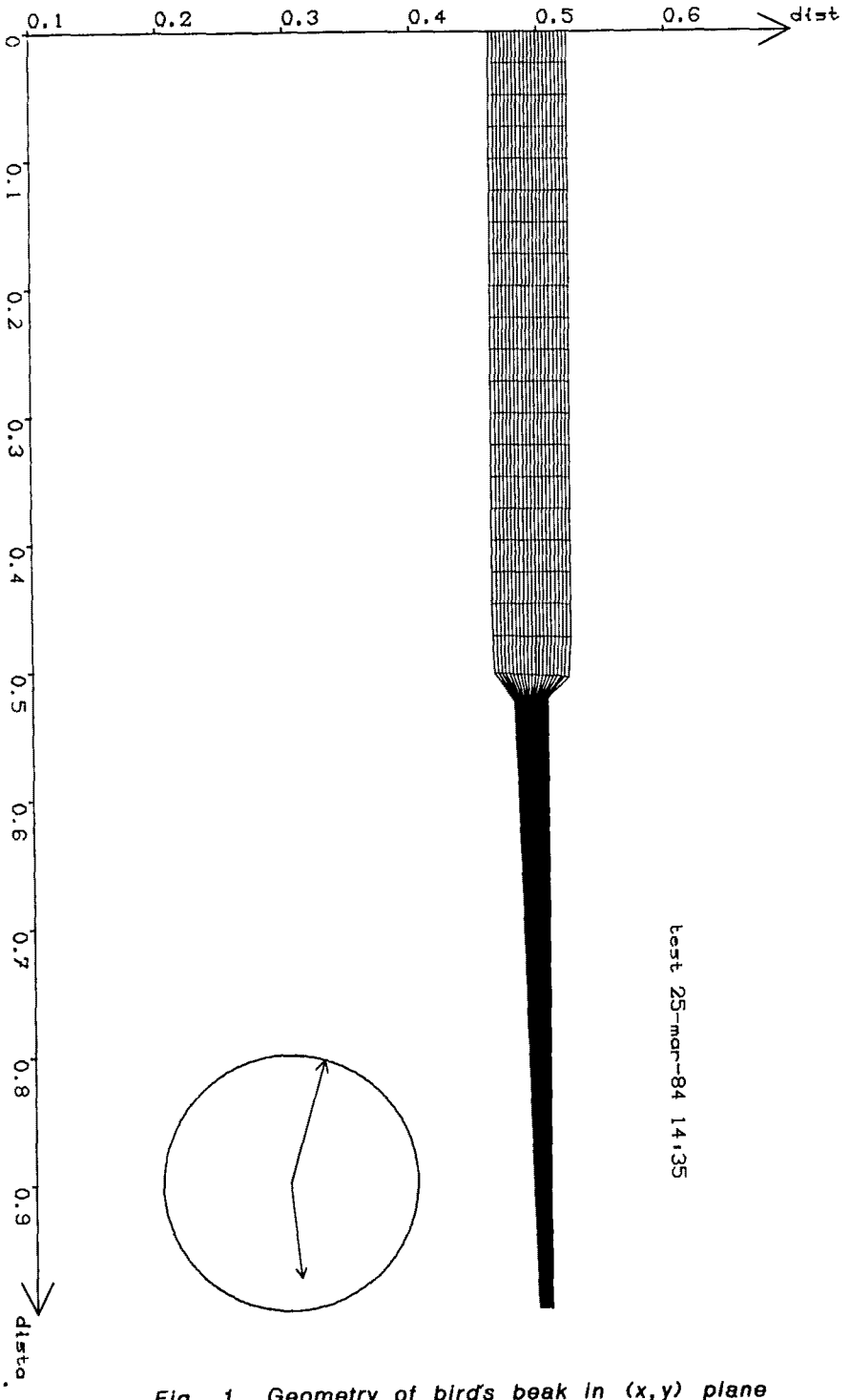

Fig. 1. Geometry of bird's beak in (x,y) plane unit of distance is μ

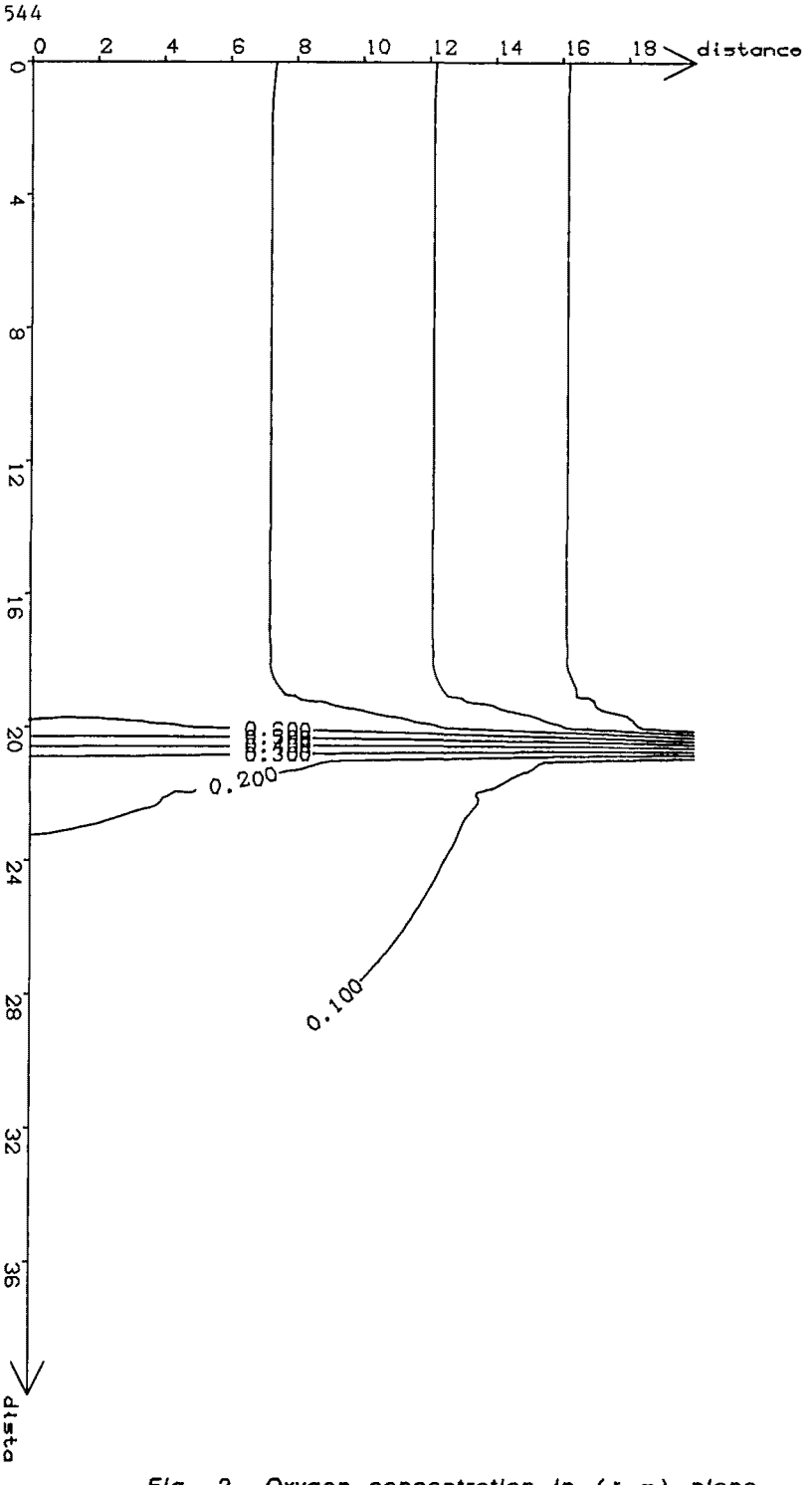

Fig. 2. Oxygen concentration in (ξ, η) plane, normalized to value of air-oxide interface

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REFERENCES

1. *Joe F. THOMPSON, Frank C. THAMES and C. Wayne MASTIN*
"Automatic Numerical Generation of Body-Fitted Curvilinear Coordinate System for Field Containing Any Number of Arbitrary Two-Dimensional Bodies"
Journal of Computational Physics Vol. 15, pp299-319, 1974.

2. *Frank C. THAMES, Joe F. THOMPSON, C. Wayne MASTIN and Ray L. WALKER*
"Numerical Solutions for Viscous and Potential Flow about Arbitrary Two-Dimensional Bodies Using Body-Fitted Coordinate Systems"
Journal of Computational Physics Vol. 24, pp245-273, 1977.

3. *Joe F. THOMPSON, Zahir U.A. WARSI and C. Wayne MASTIN*
"Boundary Fitted Coordinate Systems for Numerical Solution of Partial Differential Equations - A Review"
Journal of Computational Physics Vol. 47, pp1-108, 1982.

4. *Daeje CHIN, Soo-Young OH, Shin-Ming HU, Robert W. DUTTON and John L. MOLL*
"Two-Dimensional Oxidation"
IEEE Transactions on Electron Devices Vol. ED-30, pp744-749, 1983.

5. *Daeje CHIN, Soo-Young OH and Robert W. DUTTON*
"A General Solution Method for Two-Dimensional Nonplanar Oxidation"
IEEE Transactions on Electron Devices Vol. ED-30, pp993-998, 1983.

6. *C.W. HIRT and J.P. SHANNON*
"Free-Surface Stress Conditions for Incompressible-Flow Calculations"
Journal of Computational Physics Vol. 2, pp403-411, 1968.

7. *Michel O. DEVILLE*
"Numerical Experiments on the MAC Code for a Slow Flow"
Journal of Computational Physics Vol. 15, pp362-374, 1974.

8. *C. W. Hirt and Francis H. Harlow*
"A General Corrective Procedure for the Numerical Solution of Initial-Value Problems"
Journal of Computational Physics Vol. 2, pp114-119, 1967.

9. *Gino MORETTI*
"Importance of Boundary Conditions in the Numerical

Treatment of Hyperbolic Equations"
High-Speed Computing in Fluid Dynamics, The Physics of Fluids Supplement II, pp13-20, 1969.

10. *C.K. CHU and Aron SERENY*
"Boundary Conditions in Finite Difference Fluid Dynamic Codes"
Journal of Computational Physics Vol. 15, pp476-491, 1974.

11. *David GOTTLIEB and Eli TURKEL*
"Boundary Conditions for Multistep finite-Difference Methods for Time-Dependent Equations"
Journal of Computational Physics Vol. 26, pp181-196 1978.

12. *Tapan K. SARKAR, Kenneth R. SIARKIEWICZ and Roy F. STRATON*
"Survey of Numerical Methods For Solution of Large Systems of Linear Equations for Electromagnetic Field Problems"
IEEE Transactions on Antennas and Propagation Vol. AP-29, pp847-856, 1981.