Numerical Integral Method for Diffusion Modeling - A New Approach for VLSI Process Simulation

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Finite difference or finite element methods are traditional numerical techniques for solving partial differential equations in VLSI process simulation. Both of these approaches consume large CPU times due to fine spatial grids and small time steps required to achieve desired accuracy. In our opinion, the smooth impurity profiles in VLSI processes allow us to explore more numerically stable integral approaches to diffusion simulation. In this paper we propose a numerically efficient yet physically accurate approach which we call the *numerical integral method.* This method is an extension of the boundary integral methods[1] to solve linear and nonlinear diffusion problems with physically-based diffusivity models to account for concentration-dependent effects, oxidizing ambients effect, co-diffusion, etc.

In this method, a partial differential diffusion equation is first transformed to an integral form by using the *weighted residual techniques* with a *local weighting function* which is related to both time and spatial domains. For a two-dimensional diffusion problem, the following integral form of the diffusion equation is obtained,

$$C(x_i, y_j) = \int\int_S (W_{ij})|_{t=0} f(x,y) dS + \int_0^{t_f} \int_\Gamma (C D_{ij} \nabla W_{ij} - W_{ij}\,\mathbf{g}) \cdot d\mathbf{L} dt \qquad (1)$$

where C is the impurity concentration, S is the spatial domain, Γ is the boundary of the spatial domain, $f(x,y)$ is the initial profile, and g is the impurity flux across the boundary. On the left hand side of the equation is the impurity concentration to be calculated at a point (x_i, y_j), while on the right hand side is a spatial domain integral and a time domain integral of the impurity fluxes across the boundary.

The local weighting function W_{ij} is a solution of the *adjoint diffusion equation* with a *local diffusivity* D_{ij}. For a nonlinear diffusion problem, this local weighting function is an approximate weighting function of the diffusion equation. For example, for a semi-infinite region, a local weighting function can be written as follows,

$$W_{ij}(x, x_i; y, y_j; t, t_f) = \frac{1}{4D_{ij}(t_f - t)} exp(-\frac{(x-x_i)^2}{4D_{ij}(t_f-t)})(exp(-\frac{(y-y_j)^2}{4D_{ij}(t_f-t)}) + exp(-\frac{(y+y_j)^2}{4D_{ij}(t_f-t)})) \qquad (2)$$

The local diffusivity D_{ij} is defined as the function of the impurity concentration at the point of interested (x_i, y_j). The calculation of the local diffusivities includes the vacancy and interstitial effects as well as the built-in electrical field effect. An iterative scheme is proposed to calculate the impurity concentration based on the calculated local diffusivity. The local diffusivity is adjusted in terms of the calculated impurity concentration. The iteration stops when the difference between two consecutive values of the impurity concentration satisfies a given error tolerance. The error caused by the approximation of the weighting function is sufficiently small as long as the local diffusivities around any point do not change dramatically. This condition is valid in most practical cases in VLSI diffusion processes because the impurity profiles are smooth curves and the changes of the diffusivities cannot be arbitrarily large. In the implementation, the error can be reduced by bounding the changes of the local diffusivities.

There are several ways to compute the spatial domain integral numerically. To have an efficient integral calculation, the *Gauss-Hermite formula* is chosen with mirroring the initial profile properly on the negative half of the spatial region. For example, for a planar surface substrate, a spatial domain integral can be written as

$$S_{ij} = \int_{-\infty}^{\infty} dx \int_0^{\infty} W_{ij}|_{t=0} f(x,y) dy = \sum_{k=1}^{M}\sum_{l=1}^{N} A_k B_l F(x_k, y_l) \qquad (3)$$

with F(x,y) defined as $f(x,-y)$ for $y < 0$, and $f(x,y)$ for $y \geq 0$. Here A_k and B_l are weights, and x_k and y_l are the positions variables.

For the time domain integrals, the impurity concentration on the boundary is approximated by polynomials in the time domain, and then the numerical integration such as the *Simpson's rule* is used to evaluate the integrals.

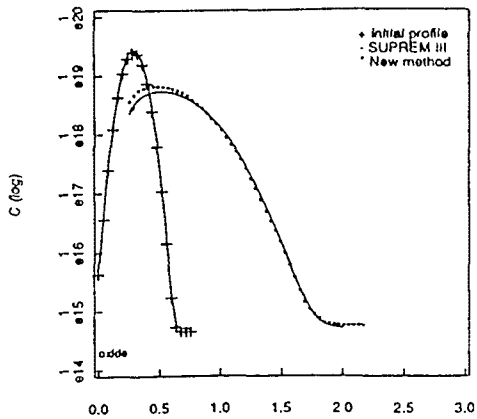
We have implemented the method for solving one- and two-dimensional diffusion problems in a computer program and run the examples on a VAXstation GPX II. The models for calculating the local diffusivities and other parameters such as segregation coefficients used in the following examples are the same as those in SUPREM III [2]. Examples 1 and 2 show the comparison of the one-dimensional simulation results between the proposed method and SUPREM III, and the execution times are shown in Table 1. The execution time for Example 3 is 52.47 seconds. Example 4 shows that the proposed method is able to handle a diffusion problem with a nonplanar surface structure.

The new method gives potential for achieving very efficient diffusion simulation. The implementation shows that very large time steps and coarse grids in numerical integration can be used to give sufficiently accurate results. The positions where the impurity concentrations are calculated can be selected for the use in the interpolation to give the initial profile for the next diffusion. Since the impurity concentrations at grid points are calculated individually, the method is naturally suited for parallel processing.

References

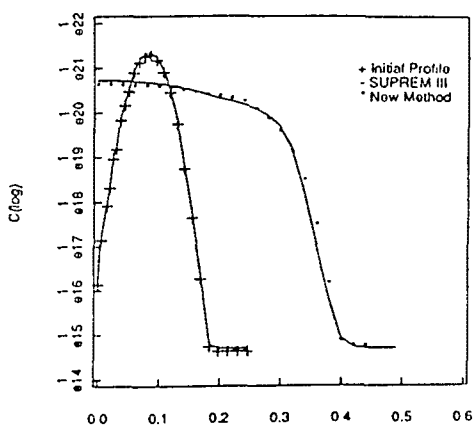
[1] C. A. Brebbia and S. Walker. *Boundary Element Techniques in Engineering.* Newnes-Butterworths, 1980.

[2] Charles P. Ho and Stephen E. Hansen. *SUPREM III - A Program for Integrated Circuit Process Modeling and Simulation.* Technical Report SEI 83-001, Stanford University, July 1983.



Example 1. Boron Redistribution
in Wet O2 Ambient

Implanted dose=5e14 cm-2, E=100 keV
Diffusion T=1000 C, t=30 min

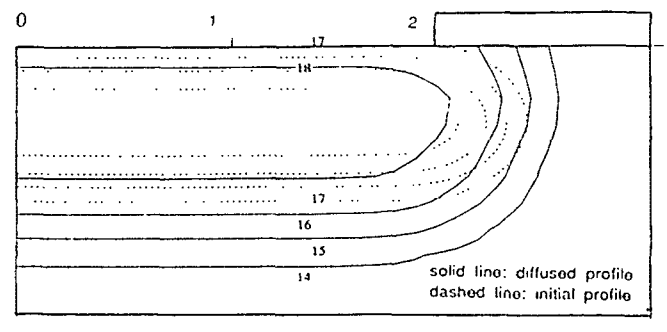


Example 2. Arsenic Redistribution
in Inert Ambient

Implanted dose=1e16 cm-2, E=150 keV
Diffusion T=1000 C, t=30 min

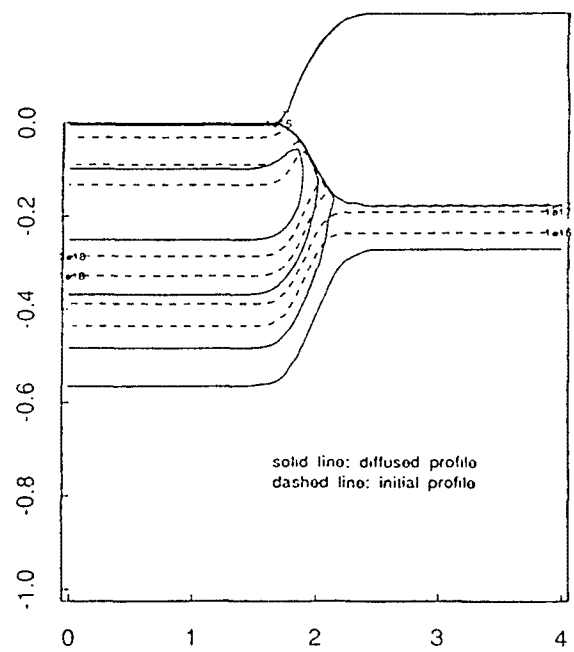
Table 1. Comparison of computation time
in 1D diffusion simulation

	Examples	SUPREM III	Numerical Integral Method
Machine execution time	Example 1	40.9 seconds	3.9 seconds
	Example 2	43.6 seconds	2.9 seconds
No. of time intervals in calculation	Example 1	44	2
	Example 2	30	3



Example 3. Boron 2D Redistribution
by Numerical Integral Method

Implanted dose=1e14 cm-2, E=100 keV
Diffusion T=1000 C, t=30 min
single time step in calculation



Example 4. Boron Redistribution
with Nonplanar Surface Structure
by Numerical Integral Method

Ion implantation through a bird's beak
dose=1e14 cm-2, E=80 keV
Diffusion T=1000 C, t=30 min
single time step in calculation