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Adaptive Mesh Refinement for Multilayer Process Simulation Using the Finite Element Method

Bruno Baccus, Dominique Collard, and Emmanuel Dubois

Abstract—An adaptive mesh refinement technique is proposed for a two-dimensional finite element multilayer process simulator. Mesh refinement is based on the dopant concentration ratio inside each element, together with a prediction technique, minimizing the interpolation errors. A significant reduction in CPU time is obtained by automatic grid refresh, several methods being tested. The mesh adequacy is evaluated with bipolar test structures using analytical punch-through voltage calculations. Applications of these methods are presented in two ways. First, an advanced trench-isolated polysilicon bipolar transistor is simulated to show the general possibilities of the techniques, and second, a coupled process and device simulation approach allows the evaluation of the scheme on real structures in relation to experimental measurements.

I. INTRODUCTION

MESH generation and refinement are key points for two-dimensional (2-D) process simulation efficiency. The simulator performance can be characterised by four elements: i) the accuracy of the solution, ii) CPU time, iii) the confidence in the physical process models, and, iv) a user-friendly interface for device simulation. For purposes of device optimization, this last point is of major importance.

However, existing tools often do not achieve good performance according to the above standard. Most codes use fixed grids for the finite difference method (SUPREM IV [1]), as well as for the finite element method (FEDSS [2], SAFEPRO [3], IMPACT4 [4]). Some attempts have been made to use adaptative grids, but the application of these techniques to complex multilayer structures has not been attempted; nor does it seem to be straightforward. Using the finite difference method, interesting work has been undertaken by Pichler *et al.* [5] for the 1-D and 2-D cases (rectangular shape). The ASWR method has also been proposed [6]. Within the finite element method, refined windows techniques have been used (TITAN [7]).

Other schemes for the finite element method have been studied, such as the refinement technique proposed by Amaratunga [8] on simple test structures, and the moving finite element has been applied to process simulation for 1-D problems [9]. On the other hand, adaptative mesh refinement is now often used in device simulation programs for general structures [10]. Finally, although there exist some theories regarding errors estimates in the finite element method [11], it is not clear whether such sophisticated techniques are needed in the case of process simulation. Moreover, the nonstationary problem arising from the simulation of diffusion makes methods of this kind not easily transportable. For example, it is expected that mesh refresh procedures might be of prime importance.

The purpose of this paper is to present numerical techniques aimed at solving these problems, taking into account the following requirements:

- Mesh generation should be fully automatic.
- Nonplanar (silicon trench) multilayer structures (doping from polysilicon) and moving boundary problems (oxidation) must be treated.
- The spatial discretization error associated with the chosen mesh must be quantitatively evaluated.
- Compared with the usual fixed grid strategy, enhanced precision should not be offset by a large increase in CPU time.

Section II describes the numerical techniques and the mesh generation principles. In Section III, simple test examples are studied in order to evaluate spatial discretization error in bipolar transistor simulation and to determine the best parameters for refinement and refresh procedure. Applications are shown in two cases in Section IV: the complete simulation of a polysilicon, trench-isolated bipolar device is first presented, and then a coupled process and device simulation makes it possible to determine the efficiency of the refinement procedure from the calculation of electrical parameters in a VLSI technology.

II. NUMERICAL TECHNIQUES AND MESH GENERATION

A. Introduction

In process simulation, the computer resources are devoted mainly to solving the diffusion equation. This nonlinear and nonstationary equation requires sophisticated techniques of spatial and temporal discretization. The support code for this study is IMPACT4, a 2-D multilayer process simulator, that uses the finite element method with linear triangular elements. The features incorporated in this program have already been described: an incomplete implicit scheme allows the linearization of the system, which is solved by the ICCG method with preconditionning [4]. Since this paper focuses on the spatial aspect,



Fig. 1. Function of mean refinement propagation, for implantation is performed on the mean (a). If all the distribution is located in the top triangle layer, only the second layer is refined (b), as no sufficient gradient is detected in the first layer. In the algorithm, if I and I2 are boundary nodes and create at least a bisection, the concerned elements are split into four ((b) and (c)). Triangles K1 and K2 have two new nodes on their sides: a third node is then added ((c) and (d)). The same procedure is used from (e) to (g) except that as I2 is an interior node creating at least two bisections (e), the concerned elements are split into four.

these techniques will not be described. On the other hand, it can be shown that, in this scheme, the temporal discretization error can be decoupled from the spatial one [12], which allows one to focus on the grid refinement techniques. Moreover, since calculated doping profiles are steeper when the mesh spacing decreases, we can determine the adequacy of the mesh by simple punch-through calculations, as will be described in Section III.

Another consideration is to examine the type of refinement to be studied: h refinement (increasing the number of elements) or p refinement (increasing the polynomial order of selected elements). In preliminary works, sixnoded triangles (quadratic shape function) were used for the diffusion problem [13], but this imposed very severe requirements on the mesh. This experience indicates that it would be difficult to extend it to a general multilayer problem. For this reason, h refinement on linear triangular elements is chosen.

B. Mesh Generation

Because of the special properties of process simulation, original procedures are introduced for mesh generation

and refinement. These are mainly based on the node connectivity limitation and also make it possible to solve the boundary consistency between different layers.

In a standard refining scheme, an element to be refined is divided into four subtriangles by adding a node at each midside. In order to obtain a conforming finite element triangulation, if one node is added on a side, the triangle is divided into two subtriangles. If two nodes are added on the sides, the triangle is always divided into four subtriangles. However, if the initial grid is very coarse, these operations may not be sufficient to obtain the correct implantation dose. Moreover a smooth transition between refined and unrefined zones is needed. For these purposes, a new "propagation" procedure, based on connectivity limitation, has been developed, as explained in Fig. 1. As this results in a propagation of the refined zones, the problems posed by the nonstationnary equations are simplified, since the diffusion front movements are anticipated. This method has been found to be more efficient in the case of process simulation than other proposed schemes [14].

In order to obtain the best triangulation, the Delaunay method is used. Here we take advantage of the MSHPTS

mesh generator from the software library of INRIA [15]. In addition, the regularization or mesh smoothing is also widely used (each node is moved to the centroid of the polygon defined by its adjacent nodes). If this latter technique is not needed for ion implantation, it is absolutely necessary for diffusion processes; otherwise the mesh quality degrades rapidly as the diffusion fronts move. On the other hand, it has the disadvantage of adding interpolation calculations. Moreover, in order to avoid very long and narrow elements, a technique based on connectivity limitation is used. Considering a patch of elements as depicted in Fig. 2(a), if node connectivity is greater than typically 11, nodes are added at the midsides of the elements (Fig. 2) in order to obtain, by a new triangulation, the structure of Fig. 2(c). Finally, the number of narrow triangles is minimized by using the technique described in [16].

In this study, it has been found sufficient, in a first approach, to apply the above procedure only to the silicon layer. The other layers then have to be updated, as the segregation phenomenon must be taken into account. (At the interface between two layers, there are double nodes at the same coordinates, belonging to each layer.) After update (new nodes being created, corresponding to the boundary added silicon nodes, followed by a retriangulation of the concerned layer), the connectivity limitation of Fig. 2 is applied iteratively. From the physical point of view, this also makes it possible to carefully take into account the extension of the segregation effect.

C. Definition of Criteria

In order to determine the regions where local refinement must be performed during the simulation, a criterion must be defined. This can be done, in the present case, with an a posteriori error estimate using local Neumann error criteria, as proposed in [17]. However this leads to supplementary calculations, and the question arises whether a simpler criterion could be as effective. To this purpose, the basic idea is that of using the concentration ratio inside each element to find out whether or not this element must be split. Such a procedure is widely used in device simulation to build the first grid but, until now, it has not been fully exploited in process simulation. By introducing the parameter α , defined below, we estimate the adequacy of a triangular element from the nodal concentration c_{ii} , for impurity i (As, B, P, Sb or other diffusing species) and node j,

$$\max\left(\frac{C_{ij}}{C_{ik}}\right) \leqslant \alpha \quad \text{with} \quad j = 1, \ 3; \ k = 1, \ 3. \tag{1}$$

However, it has been found that this criterion is not directly applicable in actual 2-D simulations because it leads to too large a number of nodes. It is then proposed that α depends on the concentration level:

$$\alpha = \alpha_0 \left(\frac{C_{\max}}{\max(C_{ij})} \right)^{0.301}$$

with $(\log_2 10)^{-1} = 0.301$ (2)



Fig. 2. Principle of node connectivity limitation technique. Considering a patch of elements, if a node connectivity is too great (a), nodes are created at midsides. The number of created nodes is half the number of node connectivity (b). A new triangulation is then performed (c) and finally a regularization (d).

with C_{\max_i} being the maximum of concentration of impurity *i* in the structure. This ensures a reasonable number of nodes; moreover, the resulting meshes are nearly regular. From the physical point of view, the diffusion coefficient is related to the doping level, giving consistency to this criterion [8].

However, in the case of smooth profiles at a low concentration level, conditions (1) and (2) are not sufficient. Another problem is not well solved by the presented method: the transition between a steep profile (arsenic emitter) and the uniform background level (arsenic epitaxy at low doping level). In order to solve these cases, a "prediction" technique is introduced as follows. The ratio between concentrations before and after diffusion step is computed for each node:

$$\beta_{ij} = \frac{(C_{ij})_t}{(C_{ij})_{t+\Delta t}}.$$
(3)

The ratio between the values of β_{ij} for the nodes contained in a patch of elements is computed and compared with a limiting value:

$$\beta = \frac{\max(\beta_{ij})}{\min(\beta_{ik})}.$$
 (4)

This β value allows one to determine regions where an important change in the concentrations is going to arise at the next time step. If β is greater than 2, nodes are added following the algorithm presented in Fig. 2.

These methods are illustrated in the case of boron implantation in a silicon trench structure, with oxide masks. A value of 5 is used for α_0 , and six iterations on the refinement procedure are needed to satisfy condition (1) in silicon. Fig. 3(a) shows the initial mesh, Fig. 3(b) the



final mesh, and Fig. 3(c) the corresponding boron contours. This is a typical example where mesh refinement is very useful, since a fixed grid would contain many more nodes to accurately describe the channel stopper region, is

D. Refresh Procedure

 α_n

as illustrated in Fig. 3(c).

It is expected that a significant increase of accuracy can be obtained by applying the algorithms and criteria presented above. However, in this case, this is achieved with prohibitive computational times. This is mainly due to the fact that node elimination is not used, since condition (1) does not seem to be adequate for this aim. On the other hand, a systematic refresh at each time step is not realistic. For this purpose a "refresh" technique has been introduced, automatically performed, and determined by the program following the evolution of dopant distribution. The mean value of α is calculated at the beginning of each time step in order to determine if a refresh procedure is needed before solving the diffusion equation:

$$\begin{array}{l} _{\text{hean}} = \frac{1}{NT} \cdot \sum_{l=1,NT} \alpha_l \\ \text{with } \alpha_l = \max\left(\frac{C_{ij}}{C_{C_{ik}}}\right) \end{array} \tag{5}$$

with NT the number of elements in silicon. When the ratio between α_{mean} at the first time step and at the current time step is greater than a given value (experiments show that 1.5 is suitable), this means that the mesh is no longer optimal: condition (1) can be satisfied with significantly fewer nodes. This is typically the case after a small number of time steps following ion implantation, the profile being more flattened near the surface. This method allows one to optimize the total number of nodes for a given value of α_0 .

From a topological point of view, a general refresh procedure has been developed for complex structures and is described in Fig. 4, where, as a test, the refresh procedure is applied to the trench structure of Fig. 3(b). The first task is that of completely eliminating interior nodes and of reconstructing a list of nodes describing the boundary. Triple points (where three boundary lines converge) and points at sharp corners are extracted as proposed in [16]. A typical distance is deduced from these new boundary points (usually, half of a fourth of the smallest spacing). Between these key points, nodes of the initial mesh (before refresh) are kept if their spacing is greater than this typical distance. A first triangulation is then performed (Fig. 4(a)). The connectivity limitation of Fig. 2 is iteratively applied to obtain Fig. 4(b). Six iterations are generally sufficient to reach convergence. This mesh is now the primitive grid where condition (1) is used, and makes it possible to obtain the structure described in Fig. 4(c). The other layers are then updated taking into account this new topology.

III. TEST EXAMPLES ON BIPOLAR STRUCTURES

A. Quantitative Error Evaluation

When conditions (1) and (2) are applied, the problem is to define a "reasonable" value for α_0 . To this end, we take advantage of the doping profile evolution and evaluate the accuracy of results in a test structure. Since the electrical characteristics of bipolar devices are very sensitive to the doping profile, a calculation of the punchthrough voltage is used. By considering a uniform doping profile within the collector, an analytical expression can be derived for the punch-through voltage $V_{\rm PT}$ [18]:

$$V_{\rm PT} = \frac{Q_{B0}^2}{2\epsilon_0 \epsilon_r q N_{DC}} \tag{6}$$

where Q_{B0} is the base Gummel number and N_{DC} the epi-



Fig. 4. Example of refresh procedure on the trench structure of Fig. 3. Internal nodes are first removed and boundary nodes recalculated. Iterations on geometrical considerations (node connectivity limitation) allows to obtain an intermediate grid: a value of 11 is used for internal nodes and a value of 6 for boundary nodes. The α criterion is then applied.

taxial doping concentration. This dose evaluation has three major advantages:

- The calculation is independent of the sophistication of the process models (as it could be by comparing simulation results with experiments). It can then be used for the assessment of process simulation programs.
- An electrical parameter is determined, but interpolation errors that occur at the interface with a device simulator are avoided.
- The calculated quantity is meaningful for process engineers.

In the case of 1-D simulation, this calculation is directly applied, and in 2-D, a cross section in the intrinsic part of the device is used.

B. Test Examples

The test structure is an npn bipolar transistor where only the emitter implantation and diffusion are simulated. In this case, errors caused by coupling of dopants are eliminated, and the intrinsic parformance of the mesh is assessed. Arsenic is implanted at an energy of 40 keV and at a dose of 6×10^{15} at/cm², followed by an annealing at 1000°C for 20 min. The resulting profile is then evaluated, and the punch-through voltage is computed, assuming a constant boron base doping of 10^{17} at/cm³, a constant collector doping of 2×10^{16} at/cm³, and a base/ collector junction depth of 0.7 μ m.

As a first test, nodes are added at each time step according to condition (1) without using the refresh or the prediction technique. The same α_0 is used for ion implantation and diffusion. Both 1-D and 2-D calculations have been performed. In the latter case, a 2 μ m by 2 μ m structure is used, arsenic being implanted in a window between 0.7 and 1.3 μ m. From these calculations, three conclusions can be reached:

- i) Point spacing of 75 Å is fine enough to obtain accurate results without refinement.
- ii) For α_0 values less than 10 (2-D calculations), the initial mesh spacing has no influence on the accuracy of results, as a consequence of the "propagation" method.
- iii) It is possible to obtain very accurate results with the refinement procedure in 2-D simulations, at the expense of a large number of nodes (about 5000 for $\alpha_0 = 3$ and 10 000 for $\alpha_0 = 2$).

We now compare the results of this test case when using different refresh procedures. Generally, the number of nodes generated after refresh is significantly lower than in the initial grid. Two alternatives can be investigated: a) the final number of nodes is not changed, and b) a constant number of nodes is considered after refresh. In the latter case, the value of α_0 is automatically decreased during the refresh procedure, its final value typically being divided by 5 to 10 compared with the user-specified value. Fig. 5 represents the CPU time needed to obtain a given accuracy (specified by $V_{\rm PT}$), the maximum number of nodes being limited to 5000. In all cases (except for the fixed grid case), the initial grid spacing is 0.5 μ m. The six curves have the following meanings:

 A classical fixed grid approach: In this simple case (rectangular domain), the number of nodes rapidly becomes the main limitation. It shows the limitations of existing schemes.



Fig. 5. CPU time needed to obtain a given accuracy (punch-through voltage) on 2-D test example. The value of α_0 for each point is indicated. To obtain a basis for comparison, the number of nodes has been limited to 5000.

- 2) The refinement technique without refresh: A high accuracy is reached only for excessive CPU times.
- The refinement technique with refresh (alternative a)): CPU times are comparable to the standard fixed grid strategy, since the number of nodes after refresh is decreased.
- 4) The refinement technique with a constant number of nodes after refresh procedure (alternative b): α_0 decreased during the refresh procedure.
- 5) Simple refresh (curve 3), with the prediction technique (eqs. (3) and 4)): This latter technique is applied at the end of the refresh procedure, when condition (1) is satisfied.
- Refresh with constant number of nodes and prediction technique.

This last curve clearly shows the efficiency of the proposed schemes for this test example, since excellent accuracy is possible even with a small value of α_0 , for low CPU time requirements. The CPU time needed for refinement and refresh is balanced by the adequacy of the doping-based mesh. In this case, the number of nodes is optimized with respect to the evolution of the doping profile. When considering the trends of silicon processing towards reduction of the diffusion cycle by the use of rapid thermal annealing, this method will appear to be very satisfactory.

From a practical point of view, the following criteria are proposed:

- Very precise results are obtained using the "prediction" method together with a refresh at the same number of nodes (α₀ value adjusted during refresh).
- In this case an initial value for α_0 of 10 allows one to simulate complex structures with a reasonable accuracy while keeping upper limited the total number of nodes. On the other hand, the required accuracy of 2-D results can hardly be reached with a standard fixed grid strategy.
- In the case of process modeling, a value of 5 allows accurate results.

IV. APPLICATIONS

A. Trench-Isolated Bipolar Transistor

Advanced bipolar devices are probably one of the most difficult structures to be handled in the field of process simulation. On the one hand, segregation effects (and the associated multilayer problem from the numerical point of view) are extremely important [4]. On the other hand, the size of the domains and the required precision on the doping profiles make it very attractive for the test of mesh refinement.

The structure simulated here is taken from [19], using real dimensions and the same processing steps. The main characteristics are: deep trench isolation (4 μ m) with boron implant at the bottom; a base coupling implant in order to reduce the emitter-to-collector punch-through current; and, finally, an intrinsic base and emitter that are diffused from the same polysilicon layer. The emitter junction depth is on the order of 500 Å and the base width is approximatively 1000 Å. In order to obtain accurate profiles in the active area, mesh refinement is necessary, since the required simulation domain is at least 6 μ m by $6 \mu m$. Following the remarks of the previous section, a value of 10 is chosen for α_0 . Three polysilicon layers (for extrinsic and intrinsic bases and trench refill) and three oxide layers (thin oxide along the trench and LOCOS, sidewall spacer), are included. Fig. 6 shows the boron contours, which exhibit good stability, for the base and the channel stopper region. This is a direct result of the refinement method, as demonstrated in Fig. 7. A medium level refinement was generated at the trench bottom, whereas a large density of triangles results in the extrinsic base region and in the intrinsic part of the device. The buried layer has also an influence on the generated mesh in the middle of the structure. Finally, the conforming triangulation between the different layers is obtained, with the minimal number of nodes outside silicon. Obviously, the refinement procedure could also be applied in these layers, but it seems to be unnecessary for predicting doping profiles. The total number of nodes is 4231, and the total number of elements is 7384 for all the layers.



Fig. 6. Boron contours. Exchange of dopants between layers is clearly seen. As mesh refinement is performed in silicon, the mesh is fine in the other layers only in the vicinity of the interfaces with silicon, in order to obtain a good description of segregation effects.



Fig. 7. Final mesh. The refined areas indicate high gradient regions, especially in the intrinsic part of the device and for the channel stopper in the bottom trench.

This example shows the superiority of adaptive mesh refinement in the case of complex structures, where a fixed grid or a window technique tend to be inefficient and difficult to manipulate by the user. In the presented simulation no user intervention is required.

B. Coupled Process and Device Approach

In order to appreciate the effects of mesh refinement in real cases, the complete simulation of a standard bipolar



Fig. 8. Gain versus collector current for different values of α_0 . A comparison with experimental measurements is also provided.

process is performed. The IMPACT package is used for this purpose. Earlier works [20] have described numerical techniques used to interface between process and device simulators, in order to minimize interpolation errors associated with layer morphology and doping distribution. In our case, process models and device simulation parameters have been adjusted in 1-D calculations and are used in the 2-D structures.

One of the most important parameter in bipolar technology is the current gain. Fig. 8 shows the current gain evolution as a function of collector current for different values of α_0 (the most efficient refresh method determined from Section III is used). A good agreement with experiment is obtained with $\alpha_0 = 5$, which is consistent with the analytical calculations of punch-through voltages. For values greater or equal to 25, the simulated characteristics are not satisfactory and hence are not displayed in this figure.

This example shows the efficiency of the method proposed in Section II, allowing 2-D results nearly as accurate as 1-D calculations. Our technique allows complex structures to be simulated, while enhancing confidence associated with process models.

V. CONCLUSIONS

A new adaptive refinement technique has been developed for process simulation. Three major issues were addressed: accuracy of results, simulation of very complex structures, and use of a refresh procedure. Moreover, owing to the simple α criterion, a CPU time reduction can be achieved compared with a classical fixed grid approach. Punch-through calculations are sufficient to tune the required parameters. Application results are shown first in the case of an advanced bipolar structure, where node optimization is of major importance, owing to the widely varying scale of length to be resolved. A coupled process and device simulation approach then shows the efficiency of the methods for the study of actual structures, in view of device optimization.

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