Contour Meshing With a One Dimensional Remeshing Scheme for the Simulation of MOS Source/Drain Diffusion

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Summary

An initial meshing and a subsequent remeshing strategy suitable for the efficient simulation of non-linear dopant diffusion in the MOS source/drain regions is reported. This meshing scheme is suitable for use with the finite element method. However, the remeshing criteria used can be used for any numerical method which is used to solve the vacancy enhanced diffusion of dopants in Silicon.

The initial mesh is constructed by using the concentration contours of the 2-D as implanted profile. Mesh spacing is chosen after making some 'a priori' estimates of the maximum diffusion which can occur during the specific anneal. As the source/drain profile evolves in time new mesh points are introduced by comparing the concentration ratio of adjacent nodes. This is an appropriate parameter as the diffusion co-efficient is proportional to concentration at most for the commonly used diffusion models. The remeshing test is only carried out along mesh lines which intersect the concentration contours and is hence a one dimensional test for a two dimensional diffusion. Application of the remeshing schemes to test problems of high concentration As diffusion indicate a halving of CPU time can be achieved when compared to a solution based entirely on a static mesh.

Introduction

With the continuing trend towards the shrinking of MOS device dimensions to achieve faster switching, accurate computer simulation of MOS devices has become an essential tool for device development. To accurately simulate device performance it is of utmost importance that the doping

profiles in the channel and source/drain regions are accurately represented. While the doping profile in the channel region can be constructed from one dimensional simulation of the fabrication process the source/drain profiles require two dimensional simulation. Two of the key process steps involved in source/drain formation are implantation and the subsequent annealing. The simulation of the diffusion which occurs during the anneal stage involves the solution of the non-linear diffusion equation:

$$\frac{\partial C}{\partial t} = \nabla(D(C)\,\nabla C) \qquad (1)$$

where c is concentration, t is time and D(C) is the diffusion co-efficient as a function of concentration. The solution of (1) can in general only be carried out using numerical methods.

Because the doping concentrations in the source/drain region vary typically over six or seven decades numerical simulation of (1) for dopant diffusion is extremely computer intensive and is to date not practical as a standard engineering tool. Much effort has therefore been made recently to reduce solution times of the problem in two domains, space and time, by altering the spatial discretization (meshing) with the time discretization depending on the time evolution of the 2-D concentration profile [1,2]. The authors have also addressed this problem and report a quick and simple method to change the meshing with time when solving (1) using the finite element method. In part the efficiency of the remeshing scheme is due to the use of an 'a priori' initial mesh [3], and in part by using a remeshing criteria which is a direct measure of the non linearity of the diffusion co-efficient [4].

Numerical Formulation

A brief outline of the finite element discretization of the diffusion eqn (1) is given below. For a triangular element a linear concentration variation in space over the element is assumed [5]

$$C_{ei}(x,y) = \alpha_m C_m + \alpha_n C_n + \alpha_p C_p \qquad (2)$$

Where C_{ei} is the concentration over the ith element, C_m, C_n, C_p are the nodal concentrations of nodes m, n, p and α_m, α_n and α_p are the basis functions associated with triangle m, n, p and given as:

$$\alpha_m = \{ (y_p x_n - x_p y_n) + (y_p - y_n)x + (x_n - x_p)y \} /2A \qquad (3)$$

where A is the area of the triangle. α_n and α_p are obtained by rotation of the subscripts in (3).

Considering the time domain, the variation of C in going from one discrete time level t^o to another t^1 is taken according to

$$\int_{t^o}^{t^1} C dt = [(1-\theta) C^o + \theta C^1) \Delta t \qquad (4)$$

where $\Delta t = t^1 - t^o$, $C^o = C(t^o)$ and $C^1 = C(t^1)$.

Now integrating (1) from t^o to t^1,

$$\Delta C = C^1 - C^o = \Delta t(1-\theta)\nabla(D(C^o)\nabla C^o)\nabla + \Delta t\theta\nabla(D(C^1)\nabla C^1) \qquad (5)$$

Integrating (5) over the spatial domain

$$\int_\Omega [C^1 - \Delta t\theta\nabla(D(C^1)\nabla C^1)]d\Omega = \int_\Omega [C^o + \Delta t(1-\theta)\nabla(D(C^o)\nabla(C^o))] \, d\Omega \qquad (6)$$

Applying the spatial discretization in (2) to (5),

$$\sum_{i=1}^{N} \int_{e_i} \{[\alpha]^T[C]^1 - \Delta t\theta[\nabla(D(C^1)\nabla\alpha]^T[C^1] \, de$$

$$\int_{e_i} [\alpha]^T[C^0] + \Delta t(1-\theta) \, [\nabla(D(C^o)\nabla \, (C^o)]^T[C^o]\} de \qquad (7)$$

where N is the number of elements and e_i the ith element.

Multiplying (7) through by $[\alpha]$ and applying Green's theorem one gets the weak formulation for the Galerkin weighted residual method, with the condition $\frac{\partial Ck}{\partial x} = 0$ and $\frac{\partial Cl}{\partial y} = 0$ along the boundries.

$$\sum_{i=1}^{N} \int_{e_i} [\alpha][\alpha]^T[C^1] + \Delta t\theta[\nabla\alpha][D(C)\nabla\alpha]^T[C^1] de$$

$$= \int_{e_i} [\alpha][\alpha]^T[C^o] \quad t\theta(1-\theta)[\alpha][D(C)\nabla\alpha]^T[C^o] de \qquad (8)$$

(8) can be expressed as a non-linear system of eqns.

$$[K(C)][C_i^1] = [Q_i] \qquad (9)$$

$i = 1,2\ldots.\ z$ where z is the number of nodes in space . (9) is then solved using either a direct or iterative method. The non-linearity due to [K] being a function of C can be taken into account by having an inner iteration using a fixed point scheme. An alternative is to use a Newton like method to solve (9). It should be noted that the choice of $\theta > 1/2$ in (8) can lead to an unconditionally stable solution of the

system of eqns (9) [6] when a constant time step Δt is used. This is an interesting observation for the finite element discretization of the diffusion equation, noting the commonly used Crank-Nicolson criteria for the finite difference discretization leads to $\theta = 1/2$.

Quasi-Linearization and Remeshing

When the differential co-efficient $[\nabla\alpha][D(C)\nabla\alpha]^T$ is used for the L.H.S. of (8), the resulting co-efficient matrix $[K(C)]$ in (9) is not symmetric. This in turn increases computer memory and processing time required to obtain a solution from (9). If for a single element the differential co-efficient is approximated by,

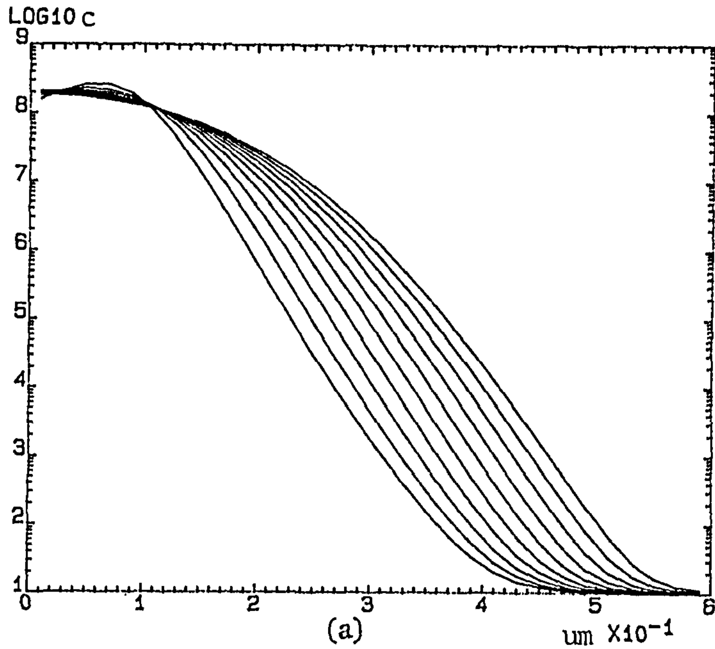
$$[\nabla\alpha][D(C)\nabla\alpha]^T = D(C_e)[\nabla\alpha][\nabla\alpha]^T \tag{10}$$

with $C_e = (C_m + C_n + C_p)/3$ then $[K(C)]$ will be symmetric. This quasi-linearisation will lead to a significant saving in computer time when the repeated solutions of (9) for inner iteration and discrete time levels are taken into account.

When solving the problem of non-linear dopant diffusion in Si it is important that the spatial representation of the dopant profile is also capable of adequately representing the product of the concentration dependent diffusion co-efficient and derivatives of the concentration. To achieve adequate representation for the non-linear diffusion over the entire time period requires either a very fine meshing or a meshing which evolves a the dopant diffuses. Fig. 1a shows a finite element solution of 90KeV, 5E15 n/cm^2 dose As implant with a constant diffusivity. When the same implant is diffused at 1000°C using a non-linear diffusion co-efficient on the same regular mesh as previously, oscilation starts to occur after $\simeq$5 mins of diffusion, Fig. 1b.

We have tried very fine time discretizations and still find that the oscillation sets in at $t \simeq 5$mins. This in turn suggests that it is the spatial discretization which is critical in simulating non-linear dopant diffusion.

Recently an algorithm for changing the meshing with time when simulating non-linear dopant diffusion using the finite difference method has been suggested [1,2]. This algorithm is based on local fitting of third order polynomials to mesh points, calculating the second derivatives from the polynomial and comparing them the numerical approximations to the second derivatives to ascertain the error in representation. This algorithm, which seems to work well for the specific finite difference formulation used has the drawback of being very time consuming as polynomials have to be fitted around each node in the x and y directions. The authors have developed a much simpler remeshing criteria which is suitable



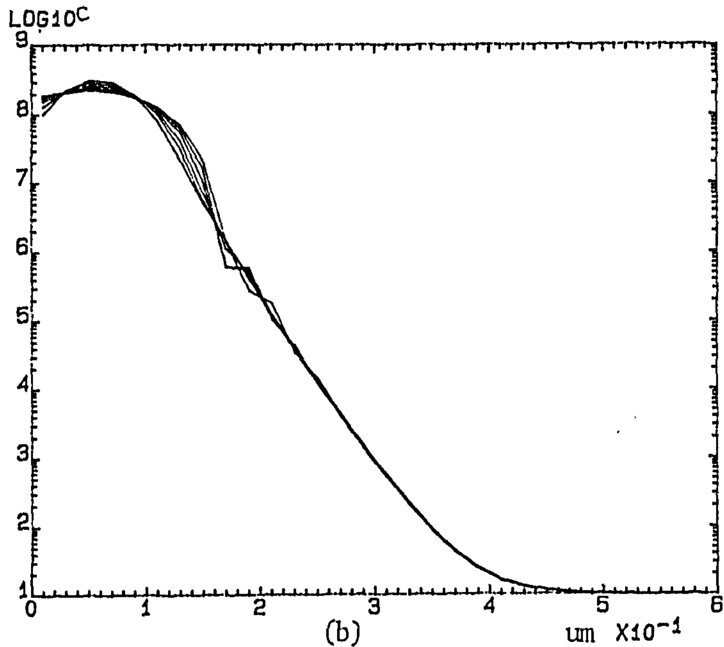


Figure 1(a)
Time evolution of a 90KeV 5E15 n/cm^2 (5E7n/um^2) As implant simulated with a constant diffusivity of 1E-5um^2/min for 20 mins.

Figure 1(b)
Spatial oscilations occuring after ≃ 5 mins of diffusion when using a non-linear diffusivity for the sample implant.

for the quasi-linear finite element formulation. This remeshing criteria is based on introducing a node when the ratio of concentration exceeds a certain value ,

$$\frac{C_i}{C_{i-1}} > \Gamma \qquad (11a)$$

and removing a node when

$$\frac{C_i}{C_{i-1}} < \frac{\Gamma}{2} \qquad (11b)$$

with $C_i > C_{i-1}$ Γ can be related to the specific diffusion being simulated,

$$\Gamma = \frac{K}{\sqrt{D_{max} \Delta t}} \qquad (11c)$$

D_{max} is the maximum diffusivity estimated from the initial implant profile and is a function of doping element and anneal temperature. Δ t is the time step. K is an empirical constant which for the quasilinear formulation has been determined as 35 x 10^{-3}um. K is akin to the empirically determined minimum allowable error of the second derivatives in the other remeshing scheme [1] described above.

Fig. 2 shows results from the application of the remeshing criteria in (11) to a 1000°C anneal of a 5E15u/cm^2, 75Kev As implant. Fig. 2a shows the initial implant with a uniform node distribution. Fig. 2b shows the result after simulating the diffusion for 20 mins at 1000°C. The mesh used was in the form of a single strip of triangular elements with all boundaries being chosen as reflective. This form of mesh proved useful in evaluating the remeshing criteria for a 2-D problem with diffusion limited to one direction. Fig. 2b shows the nodes being placed in parts of the profile where concentration changes rapidly.

This is not surprising since the test used (11) automatically builds in a test for rapidly changing regions of concentration. However, the major advantage of using (11) can be understood when the variation of diffusivity with concentration is considered. Fig. 3 shows the diffusivity of As at 1000°C including the physical effects of vacancy enhancement, electric field enhancement and clustering. Fig. 3 is obtained from the $D(C_e)$ values for each element in Fig. 2b. Also shown on Fig. 3 are D(C) values from the nodal concentrations of Fig. 2b and the projection of these nodes onto the concentration axis.

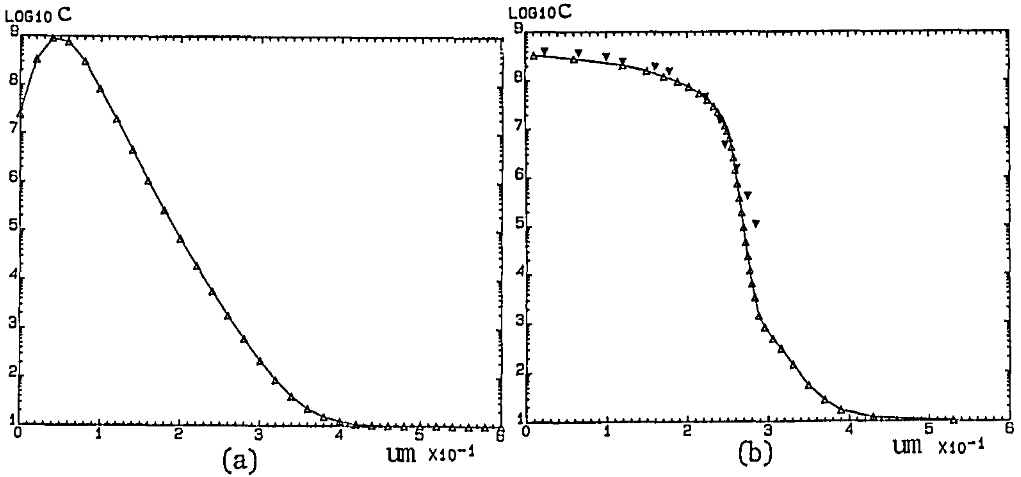


Figure 2(a)
Initial concentration and nodal distribution for a 90 KeV, 5E15n/cm^2 (5E7n/um^2) As implant

Figure 2(b)
Concentration and nodal distribution after 1000°C, 20 min anneal. (The solid symbols are experimental measurements with SIMS)

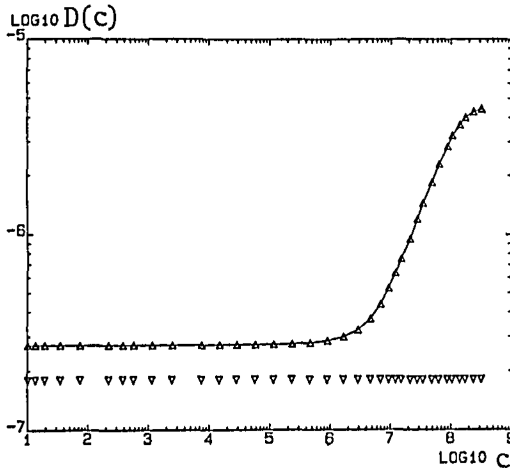


Figure 3
Diffusivity vs concentration of As at 1000°C plotted at nodal positions of the profile in Figure 2(b)

This clearly shows that most nodes are placed in regions where the diffusivity rises rapidly as a function of concentration. This rise in diffusivity is due to the vacancy enhancement and is proportional to C in the commonly used model [7]. Therefore the remeshing scheme (11) is especially suited for the quasi-linear finite element formulation as it tests not only for steep gradients in the concentration profile but also continuity of elemental diffusivity $D(C_e)$ with concentration. Fig. 4 shows a corresponding solution for a B diffusion at 1000°C.

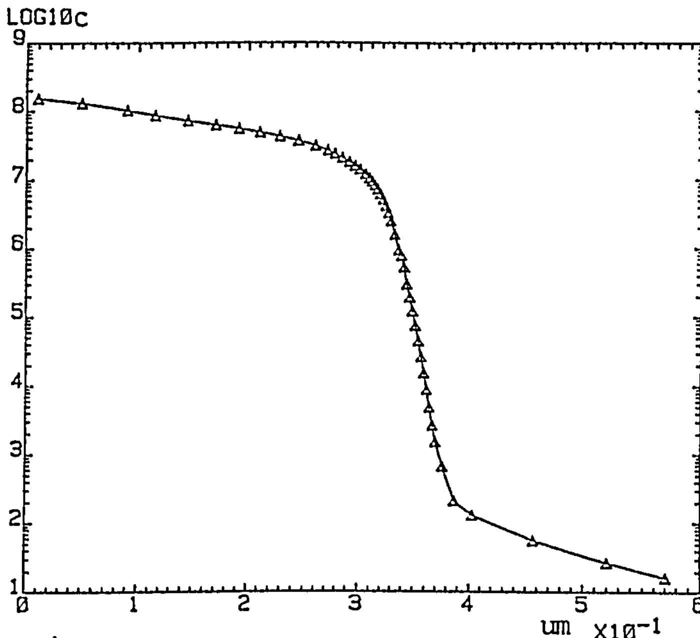
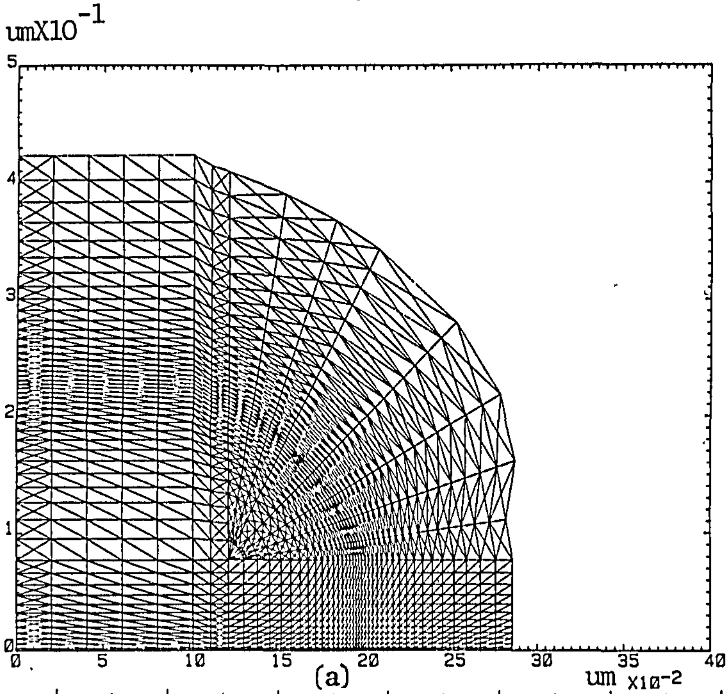


Figure 4
Profile of a 5E7n/um^2, 20KeV B implant after annealing at 1000°C for 20 mins.

Simulation of 2-D Diffusion in Source/Drains

The remeshing scheme outlined above has been incorporated into a two dimensional source/drain diffusion simulator [3], SPS-2D. This simulator has an automatic meshing scheme which is a function of processing parameters and dopant type. A typical mesh generated by SPS-2D for a $5x10^{15}n/cm^2$, 120Kev As implant which is to be annealed at 950°C for 20 mins is shown in Fig. 5a. The mesh of Fig. 5a is constructed by placing nodes along lines which are approximately perpendicular to the initial implant contours for regions beyond the projected range into the bulk silicon. The nodal spacing of the static mesh is chosen after making some 'a priori' estimates so as to have more nodes in the area where strong non-linear diffusion occurs. Full details of this meshing scheme are given in [3].



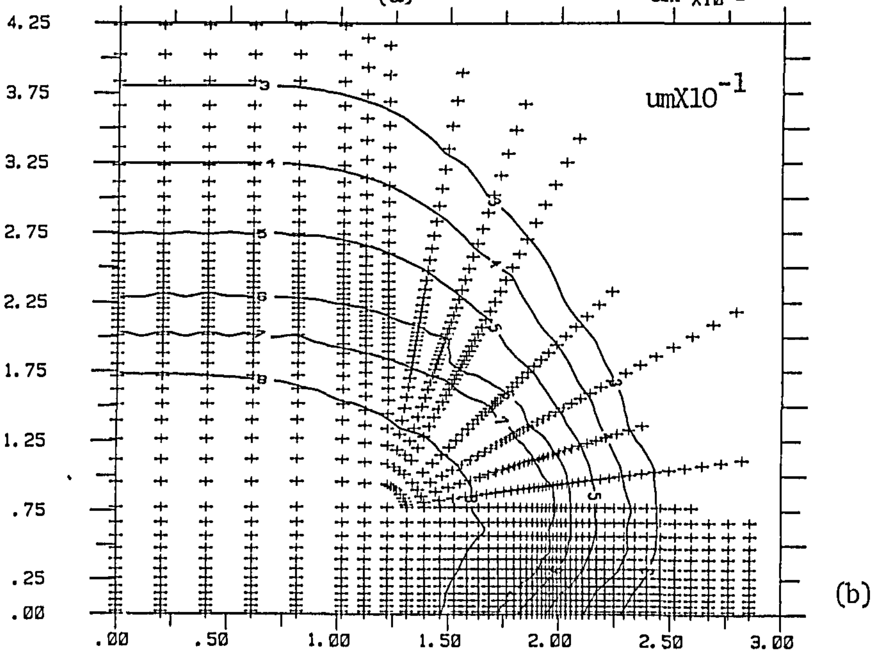


Figure 5(a)
Initial mesh generated by SPS-2D for a 5E7n /um^2, 120 KeV As implant to be annealed at 950°C for 20 mins.
Figure 5(b)
2-D profile after anneal, crosses show nodal placement. Concentration in n/um^3

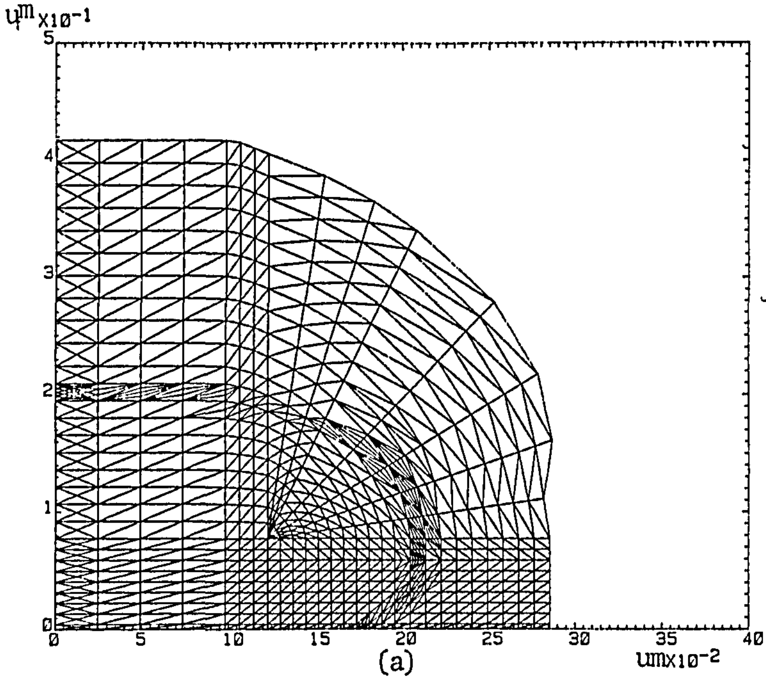
The 2-D profile after the 950°C 20 min diffusion is shown in Fig. 5b, the crosses are the node placings used. The static mesh used for the test problem had 1140 nodes, 2930 elements and with a time step of 30 secs, and the diffusion took 62 mins CPU on a Prime 750 (equivalent to VAX 780) to simulate.

The same diffusion has been simulated using the remeshing scheme on an initial mesh generated in the same manner as previously but with a reduced number of nodes placed with equispacing along the contour intersecting lines. The remeshing test was carried out only along the lines intersecting the contours. This reduced 1-D test was considered adequate for the specific contour meshing scheme used as the diffusion proceeds predominantly in a direction parallel to these intersecting lines. Fig. 6a shows the final mesh generated using the meshing scheme and Fig. 6b shows the solution for the 120Kev, $5x10^{15}n/cm^2$, 950°C, 20 min test problem.

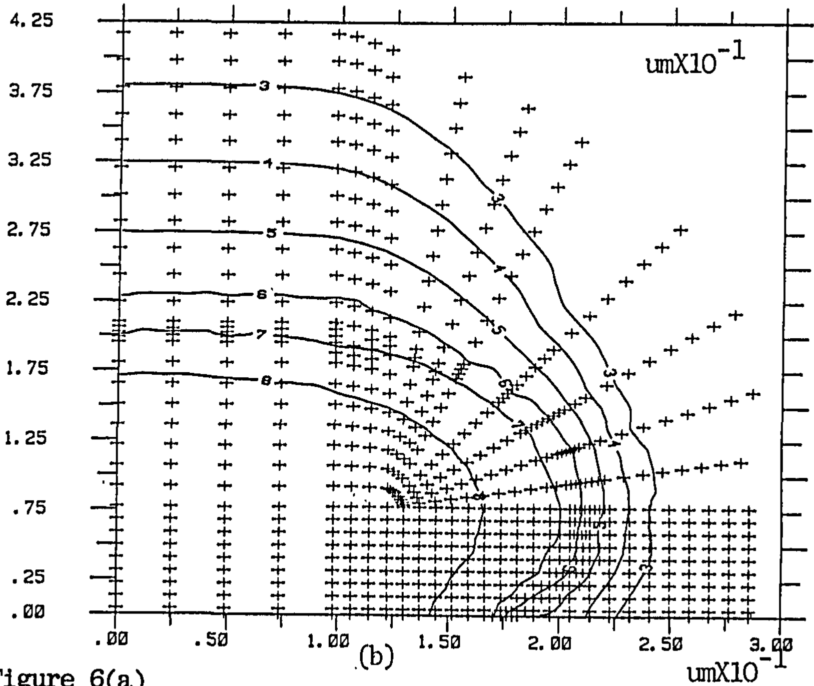
The initial mesh for the test problem had 580 nodes and 1136 elements. At the end of the solution the number of nodes and elements had been increased to 750 and 1435 respectively. No node removal according to (10b) was performed for this problem. This solution required 35 mins CPU as opposed to 62 mins using the static mesh. The time step used was 30 secs for both methods of solution. Comparing the two solution methods it is clearly seen that use of a simple remeshing scheme with initial 'a priori' meshing leads to a significant reduction in solution time.

Conclusions

A remeshing scheme which takes into account the variation of diffusivity with concentration occuring and the rapid spatial variation of concentration when simulating dopant diffusion in silicon is presented. This remeshing scheme is especially suited for a finite element formulation with a constant diffusivity for each element approximation. The remeshing scheme has been implemented for simulating two dimensional diffusion of MOS source/drain regions and resulted in a 40-50% reduction in CPU times compared with solution on a static mesh.



(a)



(b)

Figure 6(a)
Final mesh using remeshing for the As anneal (950°C, 20 mins).

Figure 6(b)
2-D concentration profile obtained with remeshing scheme. All concentration in n/um^3

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