ANISOTROPIC MESH ADAPTION GOVERNED BY A HESSIAN MATRIX METRIC

W. Wessner, H. Ceric, C. Heitzinger, A. Hössinger, and S. Selberherr
Institute for Microelectronics
Technical University of Vienna
Gusshausstr. 27-29, A-1040 Vienna, Austria
E-mail: Wessner@iue.tuwien.ac.at

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ABSTRACT

An essential task for any finite element method is to provide appropriate resolution of the mesh to resolve the initial solution. We present a computational method for anisotropic tetrahedral mesh refinement according to an adjustable discretization error. The initial attribute profile is given by an analytical function which is twice continously differentiable. Anisotropy is taken into account to reduce the amount of elements compared to pure isotropic meshes. By the proposed method the spatial resolution in three-dimensional unstructured tetrahedral meshes used for diffusion simulation is locally increased and the accuracy of the discretization improved.

INTRODUCTION

The generation of locally adapted tetrahedral meshes which carry the initial attribute profile is an important task of many modern algorithms in the finite element solution of partial differential equations, particularly for diffusion problems. The goal is to create and adapt a mesh which matches the initial attribute profile appropriately. This can only be done efficiently by anisotropic meshes.

Strict isotropic three dimensional regular meshes are not practicable for most realistic simulation structures especially in the field of semiconductor process simulation, which is our major application, because the resulting amount of tetrahedral elements required for a discretization with isotropic meshes is not practicable. The demand of calculation time and the limitation of memory require anisotropic adapted meshes which are more manageable.
The generation of tetrahedral meshes has to be enhanced by adaptation techniques where anisotropy plays a central position. The question then is how to identify these regions and how to obtain a good balance between the refined and unrefined regions such that the overall accuracy is optimal using a (nearly) minimal number of grid points. These considerations clearly show the need for error estimators which can be extracted a posteriori from the computed numerical solution and the given data of the problem. A combination of error estimation and refinement mechanism is necessary to deliver higher accuracy, if needed, by increasing the spatial resolution.

ANISOTROPIC REFINEMENT

One of the main methods for improving the spatial resolution is tetrahedral bisection which is well investigated by, e.g. (Arnold et al. 2000). When bisecting a tetrahedron, a particular edge – called the *refinement edge* – is selected and split into two edges by a new vertex, cf. Fig. 1. As new tetrahedra are constructed by refinement, their refinement edges must be selected carefully to take anisotropy into account without producing degenerately shaped elements. Bisecting a particular edge always influences the whole batch. To avoid ill shaped elements, the longest edge of the refinement tetrahedron is used as refinement edge.

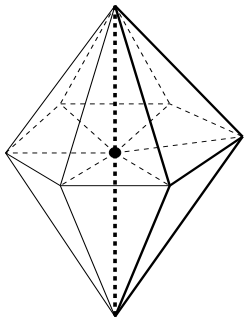

Figure 1: Bisecting.

It is obvious that the longest edge of one tetrahedron is not necessarily the longest edge of all attached tetrahedra. To bear down this problem, all new tetrahedra are directly tested and included into the refinement procedure.
A recursive approach for local mesh refinement which was suggested, e.g. in (Kossaczky 1994), cannot be applied to our situation due to the fact that anisotropy has to be taken into account.
To embrace anisotropy the basic idea of our refinement strategy is to calculate the length of an edge in a certain metric space (Lo 2001), i.e., the strain of the space varies from point to point with the consequence that the length of an edge depends on its position in the space. In case the *anisotropic edge length* is larger than an adjustable value, the edge is cut in the middle.

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A set S with a global distance function (the metric g) which for every two points x, y in S gives the distance between them as a nonnegative real number $g(x, y)$ is called a metric space. A metric space must also satisfy

$$\begin{aligned} &g(x,y) = 0 \Leftrightarrow x = y \\ &g(x,y) = g(y,x) \\ &g(x,y) + g(y,z) \geq g(x,z). \end{aligned} \tag{1}$$

Calculating the length of an edge in a metric space can be seen as calculating a line integral. In general an arc length ℓ_C is defined as the length along a curve C: $\ell_C = \int_C ds$. We define a symmetric and positive definite tensor $\mathbf{M} = \mathbf{M}(x, y, z)$ over the entire domain, representing a Riemannian metric (Lo 2001). Roughly speaking, the metric tensor $\mathbf{m_{ij}}$ determines how to compute the distance between any two points in a given space. Its components can be viewed as multiplication factors which must be placed in front of the differential displacements dx_i in a generalized Pythagorean theorem $ds^2 = g_{11}dx_1^2 + g_{12}dx_1dx_2 + g_{22}dx_2^2 + \ldots$.
A metric tensor at a point of the three-dimensional domain Ω can be represented by a 3×3 matrix $\mathbf{M}$. The length of a line segment $\overline{PQ}$ in a metric space is calculated by (Borouchaki et al. 1997)

$$\ell_{PQ} = \int_0^1 \sqrt{\overline{PQ}^T \cdot \mathbf{M}(P + t \cdot \overline{PQ}) \cdot \overline{PQ}}\, dt \tag{2}$$

where $\mathbf{M}(P + t \cdot \overline{PQ})$ is the metric at point $P + t \cdot \overline{PQ}$, $t \in [0, 1]$.

In (Yamakawa and Shimada 2000) anisotropy is defined by three orthogonal principal directions and an aspect ratio in each direction. The three principal directions are represented by three unit vectors $\vec{\xi}, \vec{\eta}$, and $\vec{\zeta}$, and in these directions the amounts of stretching of a mesh element are represented by three scalar values $\lambda_\xi, \lambda_\eta, \lambda_\zeta$, respectively. Using $(\vec{\xi}, \vec{\eta}, \vec{\zeta})$ and $(\lambda_\xi, \lambda_\eta, \lambda_\zeta)$ we define two matrices $\mathbf{R}$ and $\mathbf{S}$ by

$$\mathbf{R} := \begin{pmatrix} \xi_x & \eta_x & \zeta_x \\ \xi_y & \eta_y & \zeta_y \\ \xi_z & \eta_z & \zeta_z \end{pmatrix} \text{ and } \mathbf{S} := \begin{pmatrix} \lambda_\xi & 0 & 0 \\ 0 & \lambda_\eta & 0 \\ 0 & 0 & \lambda_\zeta \end{pmatrix}. \tag{3}$$

By combining matrices $\mathbf{R}$ and $\mathbf{S}$, we obtain a 3×3 positive definite matrix $\mathbf{M}$

$$\mathbf{M} := \mathbf{RSR}^T \tag{4}$$

that describes the three-dimensional anisotropy.

The crux of the matter is to find a suitable anisotropic tensor function which describes the stretching factors for a specific diffusion problem. Another problem is to find an error estimation which detects those regions where a higher spatial resolution is needed. An answer to these questions can be found when looking at the characteristics of the diffusion problem.

DIFFUSION

Diffusion can be viewed as the transport of matter caused by a gradient of the chemical potential. This mechanism is responsible for the redistribution of dopant atoms in a semiconductor during a high-temperature processing step. The underlying ideas can be categorized into two major approaches, namely, the continuum theory of FICK's diffusion equation and the atomistic theory (Nishi and Doering 2000). We are using the continuum theory approach which describes the diffusion phenomenon by

$$\vec{J} = -D \cdot \text{grad}(C). \tag{5}$$

$\vec{J}$ denotes the diffusion flux, D is the *diffusion coefficient* or *diffusivity*, and C is the concentration of the dopant atoms. In general, the diffusion models used in semiconductor process simulation are strongly nonlinear, because the diffusion coefficients depend, e.g., on the impurity concentration and the point defects distribution (Kosik et al. 2000). These dependences result in coupled equation systems for impurities and point defects. Additionally, chemical reactions and convection problems have to be considered in the models. However, for better understanding of our refinement method we use the linear parabolic diffusion problem which is given by (5) for the following analysis.
There are mainly two discretization schemes for PDEs in complex domains namely the *finite element* method and the *finite volume* (finite box) method. In our diffusion simulator we use the Galerkin approach of the finite element method with linear shape functions and with backward Euler time discretization (Putti and Cordes 1998).

GRADIENT FIELD

The gradient $\nabla C = \text{grad}(C)$ of a scalar field $C = C(x, y, z)$ in Cartesian coordinates is given by

$$\nabla C = \frac{\partial C(x,y,z)}{\partial x}\vec{i} + \frac{\partial C(x,y,z)}{\partial y}\vec{j} + \frac{\partial C(x,y,z)}{\partial z}\vec{k}. \tag{6}$$

We are looking for (6) expressed through local coordinates on the three-dimensional unit simplex T. The gradient of a tetrahedral discretization can be calculated by using linear basis functions (Zienkiewicz and Taylor 1989) applied to the three-dimensional unit. The coordinate transformation

$$\begin{aligned} x &= x_1 + (x_2 - x_1)\zeta + (x_3 - x_1)\eta + (x_4 - x_1)\zeta \\ y &= y_1 + (y_2 - y_1)\zeta + (y_3 - y_1)\eta + (y_4 - y_1)\zeta \\ z &= z_1 + (z_2 - z_1)\zeta + (z_3 - z_1)\eta + (z_4 - z_1)\zeta \end{aligned} \tag{7}$$

allows to map an arbitrary tetrahedron at global coordinates (x, y, z) to the unit simplex T (cf. Fig. 2) with local element coordinates (ξ, η, ζ). In matrix notation this can be written as

$$\vec{r} - \vec{r_1} = \mathbf{J} \cdot \vec{\delta}, \tag{8}$$

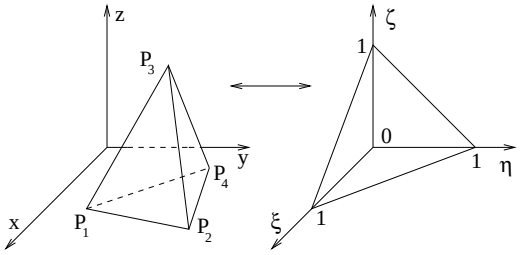


Figure 2: Coordinates transformation.

where $\vec{r} = (x, y, z)^T$, $\vec{r_1} = (x_1, y_1, z_1)$, $\vec{\delta} = (\xi, \eta, \zeta)^T$, and **J** denotes the JACOBIAN matrix

$$\mathbf{J} = \begin{pmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial x}{\partial \eta} & \frac{\partial x}{\partial \zeta} \\ \frac{\partial y}{\partial \xi} & \frac{\partial y}{\partial \eta} & \frac{\partial y}{\partial \zeta} \\ \frac{\partial z}{\partial \xi} & \frac{\partial z}{\partial \eta} & \frac{\partial z}{\partial \zeta} \end{pmatrix} \tag{9}$$

which applied to (7) results in

$$\mathbf{J} = \begin{pmatrix} x_2 - x_1 & x_3 - x_1 & x_4 - x_1 \\ y_2 - y_1 & y_3 - y_1 & y_4 - y_1 \\ z_2 - z_1 & z_3 - z_1 & z_4 - z_1 \end{pmatrix}. \tag{10}$$

Using linear basis functions on the three-dimensional unit simplex (Bauer 1994), which are given by

$$\begin{aligned} N_1 &= 1 - \xi - \eta - \zeta, & N_2 &= \xi, \\ N_3 &= \eta, & N_4 &= \zeta, \end{aligned} \tag{11}$$

allows a linear approximation of the scalar field over the element in the form

$$C_T(\xi, \eta, \zeta) = \sum_{k=1}^{4} N_k(\xi, \eta, \zeta) C_k, \tag{12}$$

where C_k denotes the scalar value of the solution on vertex k of the three-dimensional unit simplex T.
Applying (6) to the linear approximation, given by (12), results in

$$\nabla C_T(\xi, \eta, \zeta) = \begin{pmatrix} -C_1 + C_2 \\ -C_1 + C_3 \\ -C_1 + C_4 \end{pmatrix} \tag{13}$$

for the gradient of the spatial discretization element. Using the inverse of the transposed JACOBIAN matrix the gradient in global coordinates can now be expressed by :

$$\nabla C_T(x, y, z) = (\mathbf{J}^T)^{-1} \cdot \nabla C_T(\xi, \eta, \zeta). \tag{14}$$

It is in the nature of this approach that the gradient $\nabla C_T(x, y, z)$ (14) is constant over an element T and forms a piecewise constant gradient field which gives a granular approximation of the proper gradient field given by (6).
Since the vector field (14) is piecewise constant, it is obvious that strong variations of the gradient from one element to an adjacent one yield an approximation error when compared to the proper continuous gradient field. This gradient approximation error causes a diffusion flux error which gives rise to a violation of the law of mass conservation. The approximation gets worst if the changes of the gradient field are to high, i.e. the derivatives of the gradient field should be slight, or from an other point of view, refinement should take place at spatial regions with high second derivatives of the initial scalar field.

HESSIAN MATRIX

The basic idea of our refinement strategy is to use the HESSIAN matrix of the given (initial) solution for the anisotropy metric. The HESSIAN **H** is given by

$$\mathbf{H} = \begin{pmatrix} \frac{\partial^2 f(x,y,z)}{\partial x^2} & \frac{\partial^2 f(x,y,z)}{\partial x \partial y} & \frac{\partial^2 f(x,y,z)}{\partial x \partial z} \\ \frac{\partial^2 f(x,y,z)}{\partial y \partial x} & \frac{\partial^2 f(x,y,z)}{\partial y^2} & \frac{\partial^2 f(x,y,z)}{\partial y \partial z} \\ \frac{\partial^2 f(x,y,z)}{\partial z \partial x} & \frac{\partial^2 f(x,y,z)}{\partial z \partial y} & \frac{\partial^2 f(x,y,z)}{\partial z^2} \end{pmatrix}. \tag{15}$$

In general the entries of the HESSIAN matrix are possibly negative. To use the HESSIAN as metric for the refinement strategy, a transformation has to be performed. This transformation is done simply with the norm of all function derivatives. The corresponding metric can be written as $k \cdot \mathbf{m_{ij}} = |\mathbf{h_{ij}}| \quad (i, j = 1, 2, 3)$. To scale the metric a scalar factor k is used. This factor describes the maximum of the edge length in a static non-biased metric space where $\mathbf{M} = \mathbf{I}$, the identity matrix. The advantage of using the HESSIAN matrix is that it excellently reflects the curvature of the dopant profile and guarantees a good approximation in regions with high second derivatives (Gray 1998).

In our investigation of the method the HESSIAN must be given analytically which requires a twice continously differentiable initial attribute profile. It can be shown that a large class of realistic profiles can be produced by linear combinations of twice differentiable functions.

ERROR ESTIMATION

In order to measure the quality of a given three-dimensional discretization an error approximation is needed. According to the discussion of an interpolation error caused by using linear weighting functions (Johnson 1987), we calculate the linear approximation error

$$\begin{aligned} E_T = \Bigg| & \int_0^1 \int_0^{1-\xi} \int_0^{1-\xi-\eta} u(\xi, \eta, \zeta)\, d\xi\, d\eta\, d\zeta \\ & - \int_0^1 \int_0^{1-\xi} \int_0^{1-\xi-\eta} u_h(\xi, \eta, \zeta)\, d\xi\, d\eta\, d\zeta \Bigg| \end{aligned} \tag{16}$$

on a three-dimensional simplex T, where $u(\xi, \eta, \zeta)$ denotes the given analytical profile and $u_h(\xi, \eta, \zeta)$ the linear approximation over the three dimensional unit simplex T. For the diffusion problem the approximation error calculated by (16) can be seen as the diffusion particle difference over a tetrahedron. The difference is

caused by using piecewise linear functions to approximate the proper attribute profile. This approach is a usual one and suitable for sufficiently flat functions. For more strongly curved profiles the error of the approximation increases and a higher spatial resolution is needed.

EXAMPLE

Diffusion, in the sense of an IC processing step, refers to the controlled forced migration of dopants into the substrate or adjacent material. The resulting doping profile which plays a major role in the performance of the integrated circuit, is affected by temperature and time as well as the temperature-time relationship during processing. Dopant atoms can be introduced into silicon in many ways. The most commonly used methods are (1) ion implantation and subsequent annealing or drive-in diffusion, (2) diffusion from a chemical source in vapor form at high temperatures, and (3) diffusion from a doped-oxide source (SMS1988). Since ion-implantation provides very precise control of the implanted profile, it is used to replace the chemical and doped-oxide sources wherever possible and is extensively applied in VLSI device fabrication.

The most common class of functions for the approximation of ion-implantation or drive-in diffusion profiles are GAUSSIAN probability distributions which are given by

$$P(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{\frac{-(x-\mu)^2}{2\sigma^2}} \tag{17}$$

for a variate X with mean μ and variance σ^2 (Kenney and Keeping 1951). $P(x)\,dx$ gives the probability that a variate with a GAUSSIAN distribution takes on a value in the range $[x, x + dx]$.
The HESSIAN matrix (15) can then be built easily from the dopant profile approximation given by (17) and used for the anisotropy metric (4).

Such profiles can occur, e.g., after a diffusion with a constant dopant atoms dose. For a one-dimensional case this can be written as

$$N_d = \int_0^\infty C(x,t)dx = \text{const.} \tag{18}$$

This diffusion condition is referred to as *drive-in diffusion* (Shewmon 1989).

To see the essential impact of our refinement strategy we use a three-dimensional test structure. The underlying initial mesh (see Fig. 4(a)) is a coarse isotropic mesh which carries a normalized GAUSSIAN profile (see Fig. 3) which could occur, e.g., after diffusion with a constant dopant atoms dose.

Note that after a drive in diffusion process step the gradient of the concentration C vanishes at the surface (left end of the test structure, see Fig. 4(a)),

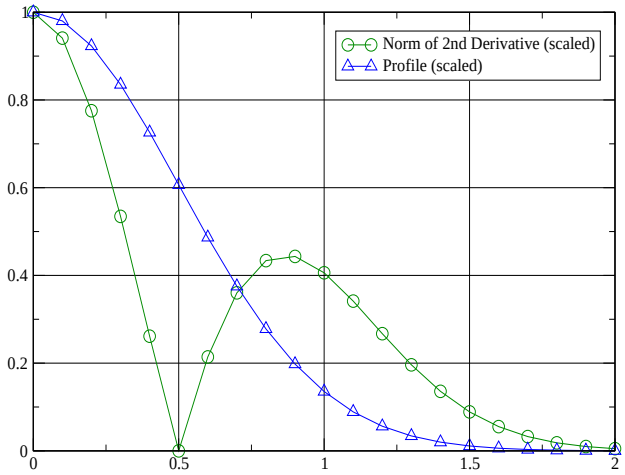


Figure 3: Test profile and norm of the second derivation (scaled to one) along the x direction of the mesh structure.

$\nabla C = \text{grad}(C) = 0$, and so does the diffusion flux $\vec{J}$ (5). Therfore the initial dopant concentration has its maximum at the left of the structure.

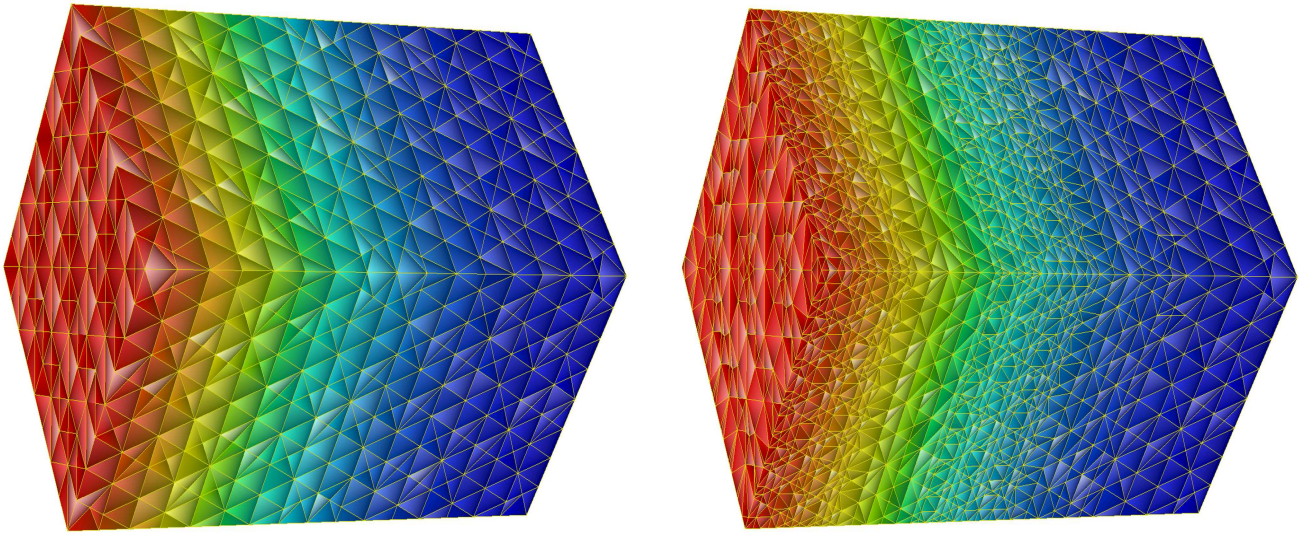
In this case the profile is one-dimensional and has therefore only one non-zero HESSIAN entry $\frac{\partial^2 f(x,y,z)}{\partial x^2}$, cf. (15). The corresponding scaled shape of the curve can be seen in Fig. 3. Using the HESSIAN matrix as input for the refinement procedure it is guaranteed that the refinement takes place where the initial solution shows a strong curvature and leaves regions with low curvature untouched.

Fig. 4(a) shows the initial coarse mesh. The tetrahedral structure is strict isotropic and mostly regular. The color of the structure corresponds to the one-dimensional initial solution which is shown in Fig. 3.

After the anisotropic refinement which is based on the HESSIAN matrix of the attribute-profile function, the refinement takes place only in regions of high curvature as shown in Fig. 4(b). The anisotropy is restricted to the x-direction of the test structure while others directions are not influenced.

Fig. 5 shows the mesh valuation according to the linear approximation error, cf. (16). We used a one-dimensional cut along the x direction through the test-structure and the error evaluation was performed along this one-dimensional cut.

At the initial mesh the error varied according to the curvature of the profile. In the regions where the profile shows a flat behavior the error is very small and therefore in this areas no refinement is needed. The shape of the error curve reflects the shape of the norm of the second derivative of the initial profile (see Fig. 3).



(a) Isotropic coarse mesh (initial mesh).

(b) Anisotropic fi ne mesh (after refi nement).

Figure 4: Mesh test structure before and after anisotropic refinement.

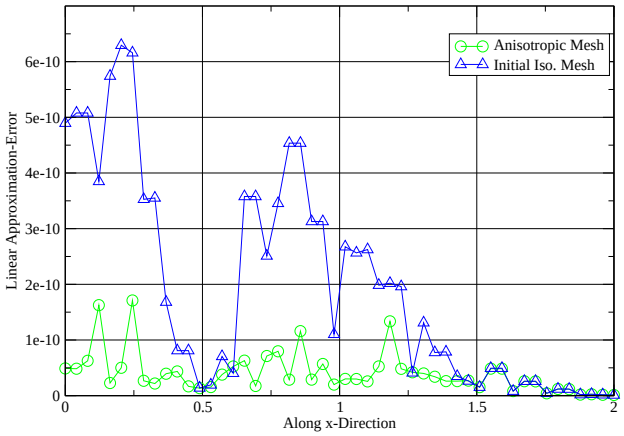


Figure 5: Approximation error E_T: one-dimensional cut through initial mesh and refined anisotropic mesh test structure.

After the refinement a rigorous reduction of the error is obtained. The variation along the x-direction has vanished and a good initial solution approximation over the whole domain was reached.

CONCLUSION

We present a computational method for locally conformal anisotropic tetrahedral mesh refinement according to an adjustable discretization error. The goal of our procedure is to create a mesh which matches an analytically given initial attribute profile appropriately. This is essential for accurate three-dimensional diffusion process simulation which is a key process of semiconductor device manufacturing.

The basic refinement step is tetrahedral bisection which guarantees a conformal mesh during refinement and allows easily local mesh adaption. A special mathematical torsion of a metric space is used to take anisotropic structures into account. This enables the reduction of elements compared to strict isotropic refinement.

It is obvious that in regions with high curvature of the initial profile the approximation error also shows high values. The refinement procedure detects those regions and uses the HESSIAN matrix of the profile for the metric space torsion. This guarantees a target oriented local mesh refinement and keeps the amount of additional mesh points small.

In our refinement procedure the initial attribute profile has to be given by an analytically function which is twice continously differentiable. At the first glance this is a loss of generality but a wide range of realistic diffusion and ion implantation profiles can be approximated with GAUSSIAN distribution functions. These function classes are continously twice differentiable and therefore perfect to form the HESSIAN matrix.

Our algorithm shows good local behavior and reflects the curvature of the initial profile excellently. The error estimations shows that the accuracy can be improved drastically by target oriented refinement. To find a good balance between refined and unrefined regions such that the overall accuracy is optimal using a (nearly) minimal number of grid points, the error estimation must be more problem oriented and reflect the nature of finite elements.

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AUTHOR BIOGRAPHIES

WILFRIED WESSNER was born in Horn, Austria, in 1977. He studied computer engineering at the 'Technische Universität Wien', where he received the degree of 'Diplom - Ingenieur' (with honors) in 2002. He joined the 'Institut für Mikroelektronik' in summer 2002, where he is currently working on his doctoral degree. His scientific interests include three-dimensional mesh generation, anisotropic mesh adaption, computational geometry, and data visualization. His e-mail address is: `wessner@iue.tuwien.ac.at`.

HAJDIN CERIC was born in Sarajevo, Bosnia and Hercegovina, in 1970. He studied electrical engineering at the Electrotechnical Faculty of the University of Sarajevo and 'Technische Universität Wien', where he received the degree of 'Diplom - Ingenieur' in 2000. He joined the 'Institut für Mikroelektronik' in June 2000, where he is currently working on his doctoral degree. His scientific interests include interconnect and process simulation. His e-mail address is: `ceric@iue.tuwien.ac.at`.

CLEMENS HEITZINGER was born in Linz, Austria, in 1974. He studied Technical Mathematics at the 'Technische Universität Wien', where he received the degree of 'Diplom - Ingenieur' (with honors) in 1999. He joined the 'Institut für Mikroelektronik' in February 2000. From March to May 2001 he held a position as visiting researcher at the Sony Technology Center in Hon-Atsugi (Tokyo, Japan). He received the doctoral degree in technical sciences (with honors) from the 'Technische Universität Wien' in 2002. In January 2003 he was awarded an Erwin Schrödinger Fellowship by the Austrian Science Fund (FWF) for the project entitled *Mathematical Models for Nanoscale Semiconductor Device Engineering.* In March 2003 he held a position as visiting researcher at Cypress Semiconductor in San Jose (CA, USA). His scientific interests include applied mathematics for process and device simulation. His e-mail address is: `heitzinger@iue.tuwien.ac.at`.

ANDREAS HÖSSINGER was born St. Pölten, Austria, in 1969. He studied technical physics at the 'Technische Universität Wien', where he received the degree of 'Diplom - Ingenieur' in January 1996. He joined the 'Institut für Mikroelektronik' in June 1996. In 1998 he held a visiting research position at Sony in Atsugi, Japan. In September 2000 he finished his Ph.D. degree at the 'Institut für Mikroelektronik' where he is currently enrolled as a post-doctoral researcher. In 2001 he held a position as visiting researcher at LSI Logic in Santa Clara, CA, USA within the scope of a cooperate research project on three-dimensional process simulation. In 2001 he also received a grant from Austrian Academy of Science within the scope of the Austrian Program for Advanced Research and Technology for his work on three-dimensional process simulation. His e-mail address is: `hoessinger@iue.tuwien.ac.at`.

SIEGFRIED SELBERHERR was born in Klosterneuburg, Austria, in 1955. He received the degree of 'Diplom - Ingenieur' in electrical engineering and the doctoral degree in technical science from the 'Technische Universität Wien' in 1978 and 1981, respectively. Dr. Selberherr has been holding the 'venia doceni' on 'Computer-Aided-Design' since 1984. Since 1988 he has been the head of the 'Institut für Mikroelektronik', and since 1999 dean of the 'Fakultät für Elektrotechnik'. His current topics are modeling and simulation of problems for microelectronics engineering. His e-mail address is: `selberherr@iue.tuwien.ac.at`.