Enhanced Advancing Front Delaunay Meshing in TCAD

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Abstract **– New developments of the advancing front Delaunay mesher *deLink* are presented. The motivation for the advancing front Delaunay method and its differences compared to the in three dimensions commonly used incremental Delaunay algorithm are shortly discussed. A new element quality assessment with regard to anisotropy and so called "flat tets" or slivers is proposed.**

I. INTRODUCTION

The advancing front Delaunay method has been introduced in [1, 2]. This method is motivated by two important advantages. First, the advancing front Delaunay algorithm is a locally confined method similar to other advancing front methods. All other Delaunay methods are not, because they require the construction of a mesh for the structure surrounding convex hull (e.g. the bounding box). Secondly, it avoids expensive intersection tests which are typically employed for advancing front methods, by using a Delaunay kernel.

Figure 1 sketches these characteristics and depicts the difference between the commonly used incremental Delaunay algorithm [3] and the advancing front Delaunay method. The incremental method which is an example of a method which is locally not confined (Fig. 1-a) maintains a triangulation of the entire domain at all times. Points can be sequentially inserted in any order, and the boundary is recovered after all points have been inserted. Figure 1-b looks the same for advancing front methods with and without Delaunay kernels. However for methods with a Delaunay kernel all elements of the advancing front are Delaunay simplices and a collision detection is therefore reduced to checking for double elements (intersections in principle do not occur).

One immediate gain of the advancing front Delaunay method is the ability to confine the meshing to a local area should the need arise for mesh adaptation during transient simulation as for example in semiconductor diffusion simulation. Not only new mesh points can be introduced, but also point removal can be handled by local remeshing of cavities (Fig. 1-c and Fig. 1-d). The incremental Delaunay algorithm allows by nature point insertion, but not removal.

Alternatively coarsening can be performed by using hierarchical meshes where the solver stores all levels of refinement. However such hierarchical methods currently only apply simple refinement schemes and are not able to allow Steiner Point refinement [4].

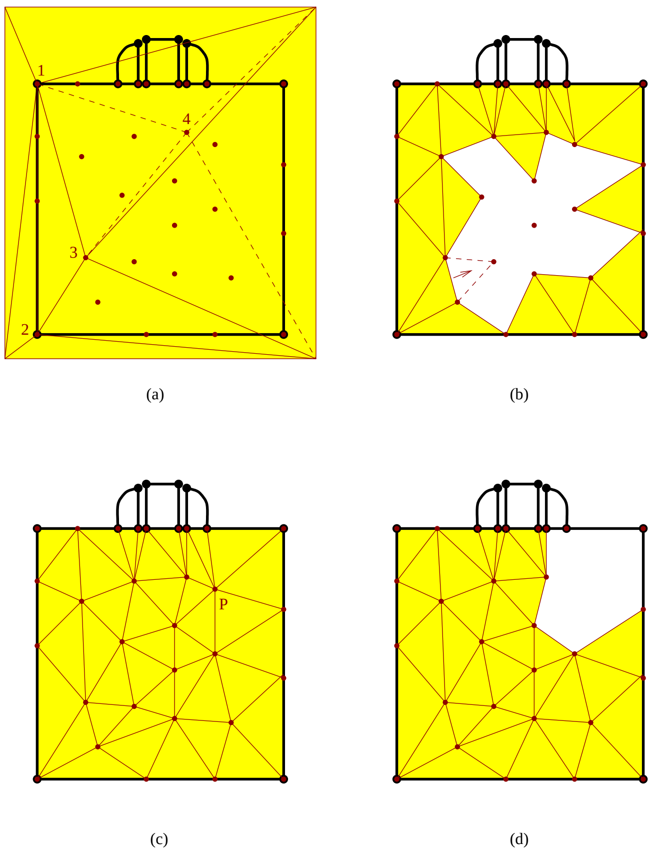

Figure 1: (a) Incremental Delaunay method with inserted points 1–3, point 4 will be inserted next. (b) Advancing front Delaunay method. (c) Point P is removed (coarsening). (d) Example of a non-convex cavity which evolves after point removal.

The discussed advantages of a combined advancing front and Delaunay method motivates its application to problems where Delaunay meshes are not required. While for finite volume discretization Delaunay meshes are required and sufficient, finite element methods motivate other quality enhancements [5]. While in two dimensions Delaunay meshes provide elements with good shape, in higher dimensions Delaunay meshes generally do not guarantee well shaped elements [6]. We present new improvements to the advancing front Delaunay method with regard to element shape quality, anisotropy, and slivers by means of Steiner point refinement.

II. PRESCRIBED ANISOTROPY

The applied state of the art in adaptive refinement methods with respect to e.g. a doping gradient is of isotropic nature. It remains an outstanding challenge to automatically adapt a mesh anisotropically and control the element quality at the same time. Edge refinement where each edge is considered separately may take the direction of the edge into account and hence should in principle be able to provide anisotropy. However, the resulting mesh quality is insufficient and a large number of obtuse angles is usually introduced. Alternatively, the refinement scheme can consider an entire element (triangle or tetrahedron) and upon refinement split the longest edge. In this way the element quality can be controlled but the refinement is isotropic again.

After ion implantation the doping is not necessarily smooth, nor has smooth gradients, and requires a highly anisotropic mesh density. A remedy to these issues is the less general approach to prescribe the desired anisotropy. It is of practical importance to construct an initial anisotropic mesh complying with mesh specifications provided by the application engineer. Such specifications include maximum element sizes given independently for different directions in a certain region.

We implemented the capability to provide such mesh spacing definitions, whereby non-coordinate-axis-aligned anisotropy and overlapping regions of spacing definitions are supported. From the possibly large set of spacing definitions for various regions one global background mesh will be extracted which holds the minimum density at each point complying with the specifications. In such a way it is fairly easy to pre-calculate a set of mesh points and thereby generate an initial anisotropic mesh. Furthermore, it is possible to achieve non-planar anisotropy near material interfaces. This is achieved by a special technique to compute the average surface normal and to allow the specification of a mesh spacing orthogonal to the material interface. However, at the moment the mesh connectivity of such boundary layers is not enforced. Such offsetting techniques have been exploited by [7].

The advancing front Delaunay method requires a priori surface meshing. The implemented surface module takes the pre-calculated points robustly into account. Points located outside the structure surface are ignored by the locally confined volume method. Points located *on* the surface are integrated into the surface triangulation resulting in a surface mesh. Points close to the surface can be snapped to the surface (projection) or deleted. The pre-calculation of points from the global background mesh avoids putting points too close to structure vertices, so no robustness issues evolve from this issue as well. Point location and snapping is performed using a point bucket octree.

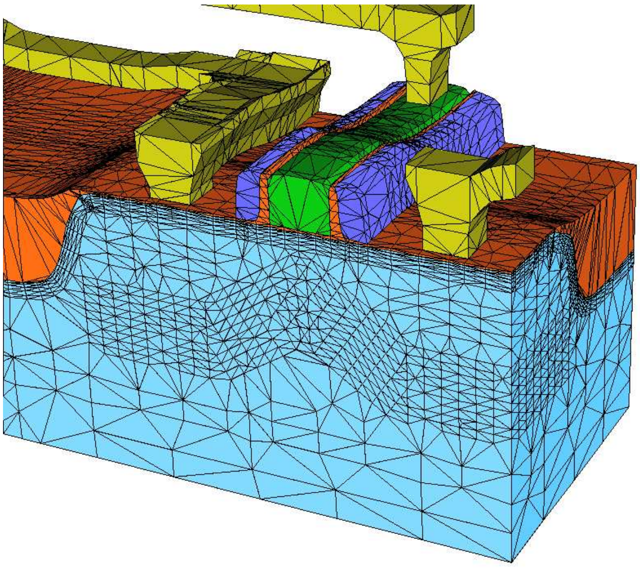

Figure 2: STI structure with 3D rounded corner and thin layer, anisotropic surface mesh (16888 triangles).

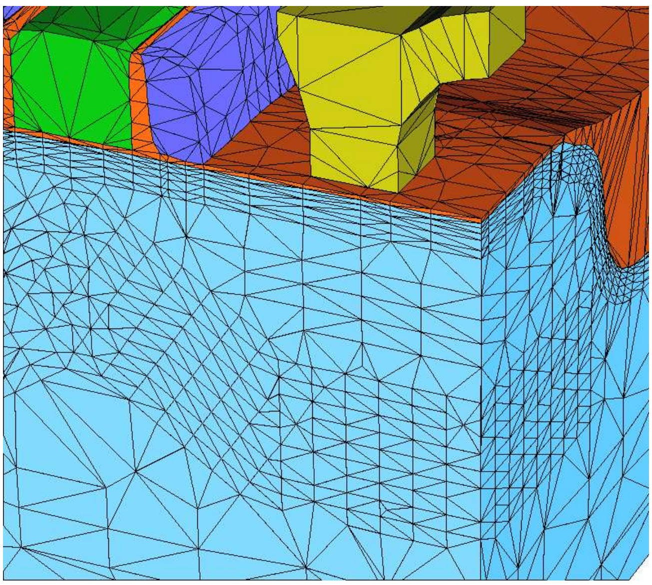

Figure 3: Region near silicon-oxide interface is shown enlarged.

Figure 2 and Figure 3 show the surface mesh for an STI structure with a fully three-dimensional rounded corner. Anisotropy near the interface and in the bulk as well as the handling of thin layers (a form of geometry prescribed anisotropy, [8]) can be observed.

III. QUALITY ASSESSMENT

Slivers are three-dimensional elements with obtuse dihedral angle and which adversely affect, for example, finite element diffusion simulation [5]. Note that slivers do not exist in two dimensions. Other types of elements with limited shape quality are depicted in Fig. 4.

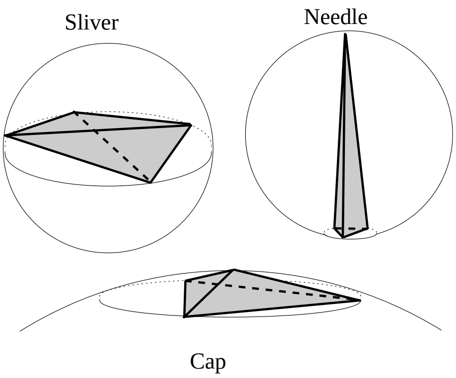

Figure 4: Fundamental element shapes in three dimensions.

Often, a single quality measure is employed to guide refinement methods to improve element quality. The measure itself is used to detect bad elements. Typical criteria for tetrahedra include

$$Q_s = \frac{l_{min}}{R} \tag{1}$$

$$AR = \frac{r}{R} \tag{2}$$

where R is the circumsphere radius, r the inner sphere radius, $lmin$ the minimum edge length, and AR the aspect ratio [9]. The problem with these criteria is that they cannot detect slivers (Q_s), or that they are not generally improved by e.g. Steiner point refinement (aspect ratio AR). Furthermore, most criteria are isotropic measures. They unnecessarily induce refinement for anisotropic elements such as needle elements which are actually desired.

We propose a new methodology whereby we first detect the *type* of element based on the number of acute and obtuse dihedral angles.

A *cap* is characterized by 3 acute and 3 obtuse dihedral angles. A *sliver* is characterized by 4 acute and 2 obtuse angles. A *needle* by our definition is characterized by 6 acute angles. Other combinations of angles indicate a mixture of the above shapes. For example, long, thin elements (needle-like) may contain 1 obtuse angle, 2 obtuse angles (sliver-like), or 3 obtuse angles (cap-like).

shape type	obtuse angles	acute angles	assessment Q_s	assessment AR
needle	0	6	low	low
cap	3	3	low	low
sliver	2	4	-	low

Table 1: Shape types, number of angles, and assessment.

The key idea is to apply different methods for different types, and to apply quality measures under the context of the type. Once the shape of an element is determined qualitatively, it is afterwards assessed quantitatively using a suitable measure. An example of type dependent quality assessment is a needle element. If a needle element has a high Q_s, AR, it is simply a normal, well shaped element. If it has a low Q_s, AR, it does not need refinement and indicates anisotropy. A cap with low Q_s can safely be refined using circumcenters as Steiner points. A sliver type element can be measured with AR and for low values requires healing.

IV. SLIVER REMOVAL

The order in which elements are processed is important, because e.g. Steiner point refinement to increase Q_s for a cap type element may produce new slivers. So sliver removal will be performed as a last step.

Currently, we perform healing of slivers with a mixed method resulting in a local transformation (tet-flip) or, if impossible, pair-wise collapsing of the 4 adjacent triangles onto each other with a following point insertion at the center of gravity to restore a consistent topology. This is still a heuristic approach and merits further investigation.

Figure 5 shows a visualization of slivers within an unoptimized volume mesh. Figure 6 and Figure 7 show the resulting volume mesh after sliver removal.

V. CONCLUSION

We implemented new features regarding anisotropy and sliver removal based on a new quality assessment methodology in *deLink*, the advancing front Delaunay mesher developed at TU Vienna. The resulting anisotropic and geometrically optimized volume mesh with improved element quality can be a basis for further doping refinement. Ideally, such a following refinement

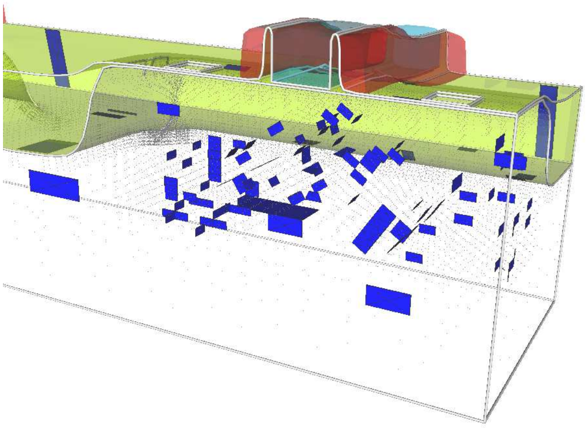

Figure 5: Visualization of slivers in an unoptimized volume mesh (131827 tets, 22585 points).

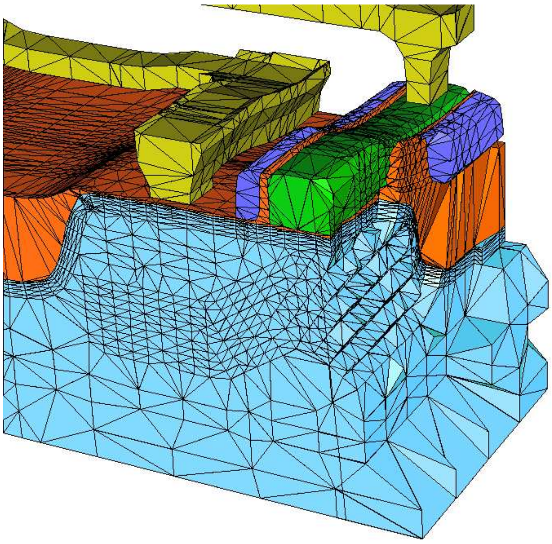

Figure 6: Optimized volume mesh visualized through clipping (131914 tets, 22622 points).

is limited to isotropic regions and does not destroy the prescribed anisotropy. Furthermore, such an adaptive doping refinement step should preserve the element quality especially if it is applied to finite element diffusion simulation.

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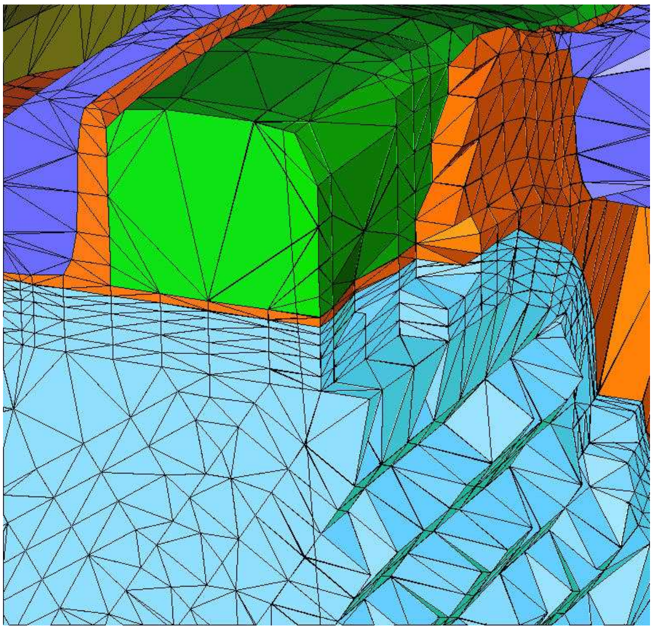

Figure 7: Optimized volume mesh enlarged.

REFERENCES

[1] P. Fleischmann and S. Selberherr, IEEE J.Technology Computer Aided Design (1997), `http://www.ieee.org/journal/tcad/accepted//fleischmann-aug97/`.

[2] P. Fleischmann and S. Selberherr, in *6th International Meshing Roundtable*, Sandia National Labs. (Park City, Utah, 1997), pp. 267–276.

[3] D. Watson, The Computer Journal **24**, 167 (1981).

[4] J. Ruppert, Journal of Algorithms **18**, 548 (1995).

[5] P. Fleischmann, B. Haindl, R. Kosik, and S. Selberherr, in *International Conference on Simulation of Semiconductor Processes and Devices* (Business Center for Academic Societies Japan, Kyoto, Japan, 1999), pp. 71–74.

[6] M. Bern and D. Eppstein, in *Computing in Euclidean Geometry*, edited by F. Hwang and D.-Z. Du (World Scientific, 1992).

[7] J. Krause, *On Boundary Conforming anisotropic Delaunay meshes* (Hartung-Gorre, 2001).

[8] P. Fleischmann, W. Pyka, and S. Selberherr, IEICE Trans.Electron. **E82-C**, 937 (1999).

[9] P. George, in *Handbook of Numerical Analysis*, edited by P. Ciarlet and J. Lions (Elsevier, 1996), Vol. IV.