A Three Dimensional Mesh Generation Method with Precedent Triangulation of Boundary

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Abstract A three dimensional mesh generation method in which triangulation of domain boundary is performed first is desirable since requirements for mesh around the boundary can be handled more easily. Based on this method, a mesh generator for 3D device simulator is developed, which can form layered mesh along planar boundary. Practicality of this simulator is demonstrated through analysis of electrical characteristics of MOS devices.

1 Introduction

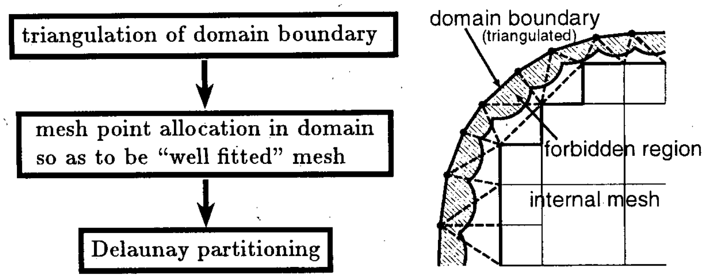
For solving partial differential equations handled in semiconductor process and device simulators, control volume method (box integration method) is widely used as descretization scheme. In order to avoid numerical instability in matrix solver, control volume method requires discretization mesh that satisfies Delaunay criterion, i.e. circumsphere of any mesh element does not contain any mesh point. In addition, near boundaries and interfaces of analysis domain, other conditions as stated below should be taken into account.

1. Descretization mesh should be "well-fitted" to the boundary, i.e. not only the mesh is conformed to the boundary, but also the circumcenter of the mesh element and circumcenter of faces of the mesh element lie in the same domain that the element belongs to. This condition should be satisfied as long as control volume method is used as discretization to avoid negative cross section associated with certain mesh edge and to avoid intuitively inappropriate control volume.
2. Layered mesh along the boundary is often necessary in order to estimate large flow along the boundary precisely [1].
3. Mesh point on the boundary should be connected with mesh point lying inside of the domain by mesh edge whose associated cross section is non-zero.

Satisfying various requirements near the boundary is hard task. For instance, most of mesh generators inserts new mesh points on the boundary afterwards in order to fulfill Delaunay criterion and make the mesh fitted to the boundary, however, this approach will make it difficult to preserve layered mesh along the boundary. Considering the difficulty in meshing around the boundary, determining the mesh around the boundary before decomposition of the whole domain will be a promising way. This paper presents a 3D mesh generation program that constructs triangular mesh on the boundary in advance. Its application to 3D device simulator is also described.

2 Overview of Mesh Generation Algorithm

As shown in Fig.1 (a), domain boundary, including internal interfaces, is triangulated at first. From this triangular mesh, "well-fitted" tetrahedral mesh is generated without adding new mesh points on the boundary, where the method we proposed [2] is utilized. The procedure of this tetrahedrization module is as follows. From the triangular mesh on the boundary, "forbidden region" (hatched region in Fig. 1 (b)) can be determined around the boundary where any internal mesh point should not be placed so that circumcenters of the mesh elements and circumcenters of faces of the mesh elements lie within the domain. This region is given as a union of hemispherical regions. By allocating internal mesh points outside of the "forbidden region" and constructing Delaunay mesh from these internal points and triangular mesh on the boundary, "well-fitted" mesh is generated. As for internal mesh point allocation, various methods can be utilized. We adopted the method based on recursive subdivision of cells [3], i.e. a box region (cell) including the whole domain is defined and is subdivided into smaller cells recursively, according to conditions given by user and conditions related to variation of impurity concentration in the cell. Apexes of cells lying out of the "forbidden region" can be used as mesh points.



(a) Basic process flow (b) Schematic view

Fig. 1: 3D mesh generation procedure.

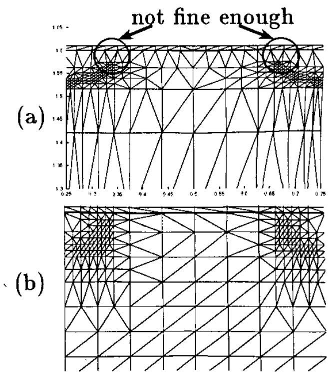
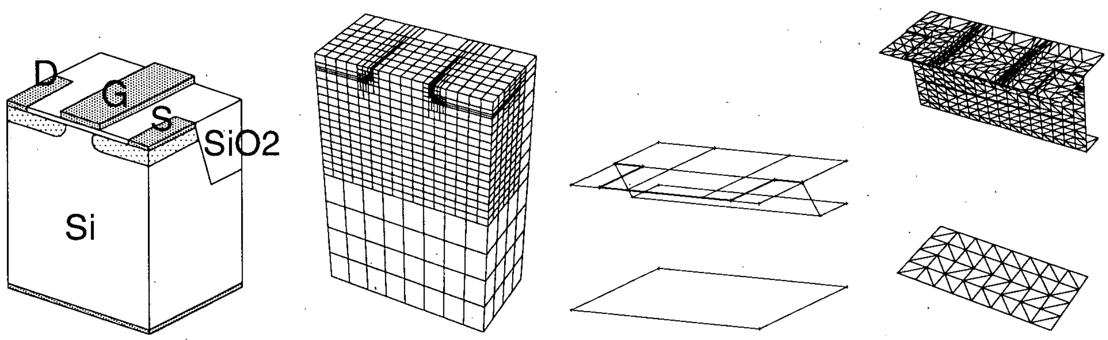


Fig. 2: Generated meshes around MOS channel region obtained from different triangular meshes on Si surface.

3 Triangulation of Boundary

Although the domain boundary is triangulated before mesh generation of internal region, size of triangular elements on the boundary should have some conformity with size of internal mesh elements. Otherwise, desired mesh point density may not be obtained due to the "forbidden region" around the boundary. Fig.2 (a) shows a mesh generated for MOS structure in case that triangular mesh on Si surface near pn junction is too coarse. Around such triangular elements, internal mesh point allocation is prohibited and mesh elements remain not fine enough. Since internal mesh point allocation is based on domain decomposition into cells, it is expected that generating triangular mesh on the boundary according to cell division will reduce the problem.

To achieve this, division of the domain into cells is performed before the triangulation. For the device structure shown in Fig. 3 (a), cell division according to impurity profile produces cells shown in Fig. 3 (b). Next, polygons which form the device structure are extracted (Fig. 3 (c)), and upon these polygons mesh points are allocated at the intersection points between polygon edges and cell faces, and between polygon faces and cell edges. Among the intersection points between polygon faces and cell edges, points too close to polygon edges are not used as triangular mesh points to avoid obtuse elements beside the edges. From available mesh points, triangular mesh satisfying Delaunay criterion is generated for each polygon by advancing front method (Fig.3 (d)). Side faces of analysis region are not extracted as polygons here since our tetrahedrization module automatically detects this boundary. Tetrahedral mesh around channel region obtained from this triangular mesh is depicted in Fig.2 (b). Fine mesh elements are placed around pn junction near Si surface in this case. Although this boundary triangulation module works well for the device



(a) (b) (c) (d)

Fig. 3: Triangulation of boundary for MOS with isolation structure. (a) Device structure. (b) Cell division. (c) Polygons extracted from the structure. (d) Triangular mesh generated on the polygons.

structure shown here, the final tetrahedral mesh may not be "well-fitted" to the boundary in general. In order to ensure this, mesh points on the boundary must be adjusted so that no point on the boundary lies in "forbidden region." This problem often occurs when device structure includes oblique thin layers. Adding new mesh points on the boundary followed by local refinement of triangular mesh will be needed to solve this problem.

4 Decomposition of 3D Domain

As described in previous section, analysis domain is basically subdivided into cells. Cells with high aspect ratio are allowed so that mesh point density can be raised with respect to certain axis. This means that dividing a cell into 2, 4 or 8 cells is possible. Because of this feature, number of mesh points can be reduced in comparison with the original octree based method.

Available mesh points for final tetrahedral mesh are apexes of cells outside of "forbidden region" and triangular mesh points on the boundary. Since a set of mesh points is given, advancing front method [4] can be applied for domain decomposition into tetrahedra, and no new mesh point is added during the tessellation process in principle. In advancing front method, tetrahedral elements are cut out from the domain one by one, however, polyhedra that cannot be divided into tetrahedra can remain in case that co-circular points exist [4]. In order to make the decomposition process stable, tessellation of cells and tessellation around the boundary are performed separately. Only cells that have no nodes in the "forbidden region" are chosen and divided into tetrahedra, and the remaining region around the boundary is tessellated afterwards. Cell can have many co-circular point sets. However, even if all the possible ways to cut out tetrahedron are tried, it will not be much time-consuming since number of mesh points in one cell is limited. In fact, processing time needed for tetrahedrization of cells is quite small in comparison with that needed for tessellation around the boundary. In addition, a heuristic technique to increase stability is incorporated, in which cutting out a tetrahedron whose apexes are chosen from the co-circular point set is delayed.

Fig.4 shows the final mesh generated by the tetrahedrization module, for the structure shown in Fig.3. Although mesh around MOS channel region is fine enough in this example, more practical mesh will be obtained by specifying desirable cell size or by adding layered mesh described in next section.

5 Application to 3D Device Simulation

Tetrahedral mesh generated by the method explained in previous sections can be passed to our device simulation program. Fig.5 shows nMOS drain current variation in slope of isolation for two different isolation structures. Negative substrate bias V_{sub} is applied to make reverse narrow channel effect clearer. As is expected, due to the leakage current near edge of the channel, larger drain current is observed as slope of isolation gets steeper (smaller θ, depicted in inserted illustration in Fig.5) for both isolation structures. Recessed LOCOS structure gives larger leakage current since more field lines must be terminated at charges

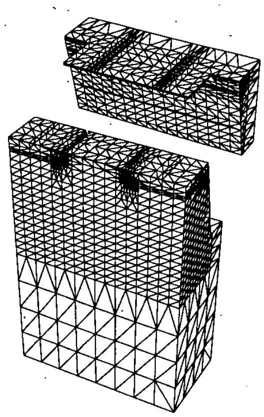


Fig. 4: Tetrahedral meshes for Si and oxide regions obtained from boundary mesh shown in Fig.3 (d).

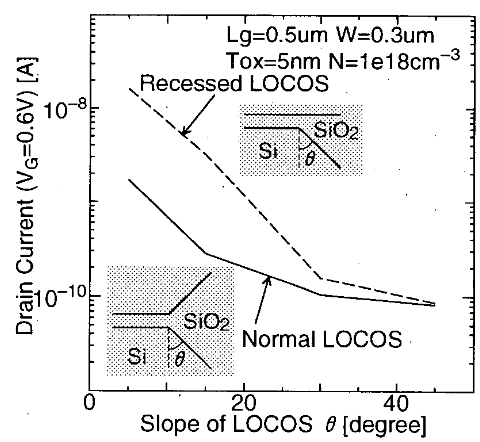


Fig. 5: Calculated drain current variation in slope of isolation. $V_d = 0.2$V, $V_{sub} = -0.5$V.

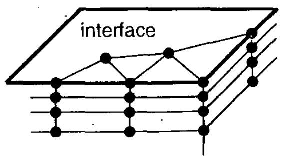


Fig. 6: Protection of interface by layered mesh, which is expected to be formed while tetrahedrization of the region.

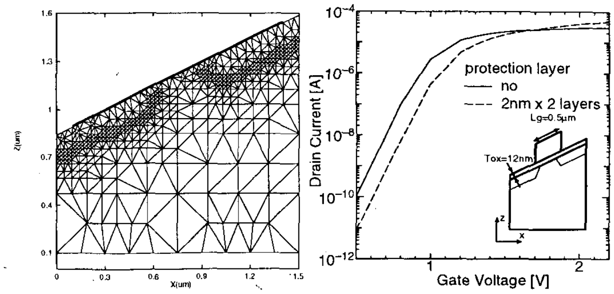


Fig. 7: Generated mesh (left) and calculated $I_d - V_g$ characteristics for MOS with oblique surface (right). Device structure is uniform with respect to y axis.

in the channel edge region. As described above, qualitatively reasonable result is obtained.

An important advantage of our mesh generator is that layered mesh along the boundary can be formed right after the triangular mesh generation. Since the triangular mesh is determined before tetrahedrization and no mesh point is added during the tetrahedrization process, the layered mesh structure is preserved. At present, quite simple method, which is effective only for planar boundary, is incorporated. After the triangulation of the boundary, new mesh points are placed at the position certain distance away from the mesh points on the boundary, so that layered mesh is expected to be generated as shown in Fig.6. Shift of "forbidden region" into the domain due to the layered mesh is taken into account during allocation of internal mesh points.

For nMOS with oblique Si surface, effect of the layered mesh is evaluated. Fig.7 shows generated mesh structure and calculated $I_d - V_g$ characteristics, where solid line and broken line correspond to the result by mesh without layered mesh and mesh with layered mesh, respectively. When the surface is protected by layered mesh, drain current in high gate voltage region becomes larger because underestimate of current flow along Si surface due to detour of the current path is avoided as pointed out in [1]. On the contrary, drain current in low gate voltage region becomes smaller since the effect of refinement of the mesh near the surface [5] is dominant.

6 Summary

A 3D tetrahedral mesh generator which determines triangular mesh on the boundary in advance is developed and incorporated into our device simulation program. This generator allows adaption to impurity profile and interface protection by layered mesh, which makes it practical and applicable to various device structures.

Acknowledgement

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