Chapter 1

Introduction

1.1 Background

The use of TCAD software has experienced a major shift in the last decade. Tools such as semiconductor device and process simulators are no longer viewed as research tools available only to university scientists and industrial researchers. As powerful workstations are easily accessible, device and process simulations have become a routine exercise for engineers to conduct the process integration, device analysis, circuit characterization and yield optimization. The proliferation of TCAD tools has a significant economical impact on the semiconductor industry. First, the shortening of the design-to-manufacture time for new products mandates a rapid design cycle for bringing up new technologies. An effective use of TCAD tools saves much experimental time for calibrating process and device parameters and minimizes the number of the trial-and-error iterations. Second, the skyrocketing cost of modern IC fabrication facilities forces engineers to re-evaluate the methodology for new technology development. Advanced simulation capability greatly reduces the cost by (i) detecting design flaws in the early design stage and (ii) achieving optimal solutions through parameter calibration. Third, yield optimization has become the single important factor for reducing the product cost. TCAD tools play a significant role by dynamically optimizing equipment parameters during the manufacturing process.

The shift of TCAD tool users poses a challenge for the tool usability. In the past, the user community consists mainly experts with good understanding of the computational models deployed by the TCAD software. With the knowledge of numerical algorithms and physical models, expert users are capable and willing to do everything necessary to make tools work. However, as more non-experienced people are engaging in the use of TCAD tools, it is unrealistic to expect these users having the same knowledge level.

The difficulty of the usability is due to the difference of the functionality of a tool perceived by the users and the computational model implemented by developers. For example, the objective for a device simulator user is to understand the behavior of a device with different characteristics and under various bias conditions. From the implementation viewpoint, a semiconductor device is modeled through a geometric structure with certain physical properties which are governed by a set of partial differential equations. To implement a device simulator, first we need to describe the geometric structure of the device. Then we discretize the geometry region. Finally we solve the PDE system by applying some numerical schemes, such as the finite difference method or the finite element method.

The implementation aspect of a tool has little interest for most TCAD tool users. Ideally, the computational model of a TCAD tool should be encapsulated from the tool users. However, such an encapsulation layer does not exist for many of today's TCAD tools, which handicaps the tool usage. As semiconductor problems become more complex and computational algorithms more sophisticated, the usability becomes a more severe problem. Some efforts have been made in the last several years to address the problem. In this thesis, two usability issues are studied: (i) the automation of mesh generation and (ii) a 3D informational model for device simulation system.

1.2 Related Research Activities

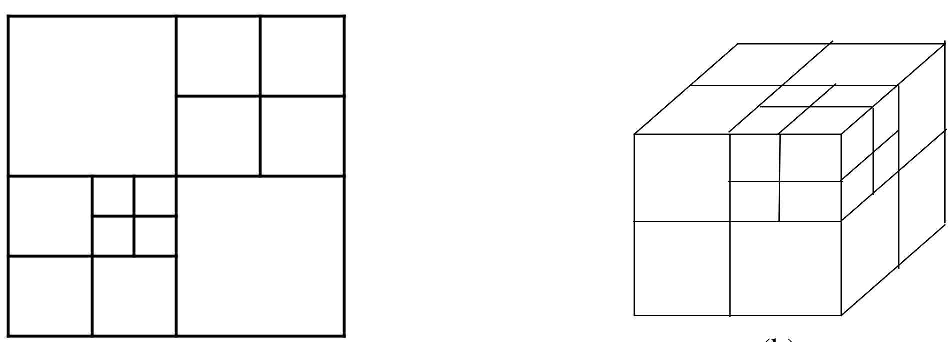
Mesh generation and the information model for the semiconductor device simulation constitute the main body of the thesis. A brief overview of some related research activities are presented in this section. The objective is to highlight the research issues that are being addressed in this study.

1.2.1 Mesh Generation

Spatial decomposition is the technique which recursively decomposes a geometry domain into sub-regions. Two commonly used techniques are the quadtree in 2D and the octree in 3D, as illustrated in Figure 1.1. The technique has been successfully used for solving problems of graphics and computational geometry. In the early eighties, Shephard and his colleagues introduced the quadtree-based technique for mesh generation [YERR84]. One problem with the early version of the quadtree mesh generator is its difficulty in handling the boundary of a mesh region. The vertices of the boundary were always snapped onto quadrant vertices. Hence, the resulting mesh region is an approximation of the original region. Depending on the size of quadrants, the difference between the problem domain and the approximation region.

Due to the regularity in structure, a 2D quadtree based mesh scheme can be extended to 3D mesh generation using an octree decomposition [YERR84, PERU89]. A main difficulty for the 3D octree mesh scheme is tetrahedralization, specially for generating quality elements along the boundary. Different schemes have been proposed and most are based on tetrahedron removal techniques [WOO84, ALUR92].

In this thesis, a modified tree based mesh algorithm is proposed which is applicable to both 2D quadtree and 3D octree mesh generation. Two new features incorporated are the level control function and the δ-zone triangulation. The level control function provides a way of controlling the mesh density and guarantees the balance of the tree. The δ-zone



(a) (b)

Figure 1.1 Illustration of spatial decomposition: (a) quadtree decomposition. (b) octree decomposition triangulation improves the quality of the mesh elements along the boundary of the mesh domain.

1.2.2 Mesh Generation for TCAD

The device simulators such as PISCES and STRIDE [PINT84, WU90] use the control volume method for solving a system of partial differential equations. Similar to the finite element method, the control volume method can be applied to an unstructured triangular mesh. When the geometry structure of a device is fairly regular, manual generation of the mesh is a feasible solution. As semiconductor devices become more complex, it becomes a very time consuming and error prone task for the novice users. An early employment of the automatic mesh generation for 2D device simulators was the adoption of TRI, a mesh generation module from PLTMG, a PDE numerical solver package[BANK90]. The mesh scheme for TRI is based on the recursive partition of a mesh domain with triangles. In the process of the triangulation, edge swapping technique is applied if ill-shaped triangles are detected. One drawback with TRI is its difficulty to control the mesh density, specially inside the diffusion region.

A different 2D mesh generator called MESHBUILD was later developed at ETH [MULL92]. MESHBUILD was based on a 2D rectangle decomposition technique and was able to generate unstructured mesh with no obtuse angle elements. In MESHBUILD, the mesh density is controlled by the variation of the doping profile so that a denser mesh can be generated around the junction area, which is very desirable for most device simulators. A major difference between the MESHBUILD and some other 2D quadtree based mesh generators is that MESHBUILD partitions the entire mesh region into a set of rectangles and then applies the spatial decomposition recursively on each of the rectangles. The advantage for taking such an approach is that no vertex moving step is required during the triangulation step. However, excessive number of elements could be produced, especially when some parts of the region boundary exhibit many irregular “zigzags”.

For 3D unstructured mesh, one type of schemes is to use prisms for the elements. This approach has been used in both FIELDAY-3D and DAVINCI [BUTU81, TMA92]. A prismatic mesh is generated by extruding a 2D triangle in the third dimension. The advantage for such an approach is that any 2D triangular mesh algorithm can be adopted with little effort. However, for many semiconductor devices, a prismatic mesh is not sufficient to accurately represent the device geometry. For example, a cone-like polyhedron cannot be meshed with only prism elements, as illustrated in Figure 1.2.

A 3D octree based mesh generator, OMEGA, was developed at ETH [CONT90]. In OMEGA, the mesh density is controlled by the variation of the doping profile. The tetrahedralization scheme is based on a predefined pattern matching approach, i.e. only certain patterns of octants can be tetrahedralized. Because of this constraint, the boundary of a mesh region can only be approximated. In order to achieve accurate approximation, many small octants are required for a “non-smooth” boundary.

Recently, a new version of OMEGA, OMEGA_M, was developed at ETH [HITS93]. OMEGA_M decomposes the mesh region into a set of pre-defined geometry primitives, such as bricks, prisms and pyramids. Depending on its shape, each primitive is recursively refined. The advantage of the approach is that complex tetrahedralization step is not required. However, it imposes more constraints on a mesh region.

1.2.3 TCAD Framework

A good overview about various TCAD framework activities can be found in the thesis by Wenstrand [WENS91]. Since 1990, a major effort, organized by the TCAD subcommittee of the CAD Framework Initiative (CFI), has been launched to develop an industrial standard for the TCAD framework. An object-oriented information model, Semiconductor Wafer Representation (SWR), has been proposed as a unified information model for a wafer state. SWR consists of two information servers, the geometry server and the field server. The geometry server provides the geometry information about the wafer and the field server provides the physical properties. The SWR version 1.0 has been prototyped in 1991 and was officially approved in 1993 [CFI93]. A recent development of the version 1.5 extends the informational model to include 3D models. The second part of

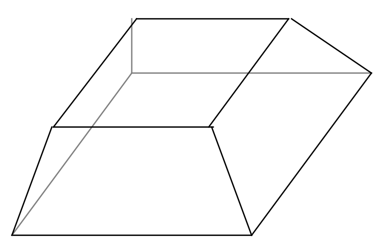


Figure 1.2 Cone-like 3D region.

the thesis describes a prototype implementation of the information model based on the SWR1.5.

1.3 Research Objectives

The objectives of this thesis are summarized as follows:

> *(i) To identify the requirements for mesh generation and to formulate a mesh generation strategy suitable for the semiconductor device simulation.*
>
> *(ii) To explore interrelationship among components of a TCAD framework, including the information model, services and application tools.*

The study of a meshing scheme suitable for semiconductor device simulation involves issues such as mesh optimality, algorithm development and complexity analysis. To understand the informational model for the TCAD framework, we need to abstract a minimal but complete set of information for TCAD tools, to develop a general but flexible schema for accessing the informational model and to implement the services around the information model, which are necessary for the framework to be usable. In addition, the issues related to the software design and implementation are also addressed, which include the architecture analysis, programming techniques and software testability and reusability.

1.4 Thesis Outline

This thesis is organized as follows:

Chapter 2 presents an overview on the different meshing schemes used for the solution of partial differential equations. Different meshing schemes are grouped according to the complexity of the supporting data structure, i.e. structured, unstructured and semi-structured. In addition, a review of the requirements imposed by the numerical solvers as well as the semiconductor device simulation is presented.

Chapter 3 describes the 2D quadtree based meshing algorithm. Two new concepts are introduced, the level control function and the δ-zone. The level control function is used to generate a balanced quadtree and the δ-zone separates the boundary region from the interior region so that a more sophisticated triangulation scheme can be applied to the regions near the boundary to prevent generating ill-shaped triangles. With these two enhancements, a quality mesh for both the interior region and the region near the boundary can be generated. In addition to the detailed discussion on the computational algorithms, a theoretical analysis on the mesh optimality is provided.

Chapter 4 discusses the extension of the computational algorithms presented in Chapter 3 for the 3D mesh generation. First, the implementation of the algorithms for the 3D mesh generation are discussed. Then, the chapter focuses on the development of the tetrahedralization algorithms.

Chapter 5 discusses the issues regarding to the information model and the TCAD framework. In addition to the extension of the SWR to the 3D device models, various services provided by the framework are described, which include the geometry modeling service and the mesh service.

Chapter 6 discusses the implementation issues of mesh generation. A detailed discussion about the object-oriented technique is presented with its application to the implementation of the 3D mesh generator. A prototype implementation of a 3D device simulation system is also presented. The implementation of the information model, the services and several applications are examined.

Chapter 7 concludes the thesis with a short summary of contributions and a discussion on the future work.