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Recursive M-Tree Method for 3-D Adaptive Tetrahedral Mesh Refinement and Its Application to Brillouin Zone Discretization

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Abstract

We present a high speed adaptive tetrahedral mesh refinement method based on the Recursive Multi-Tree algorithm. To our knowledge, this is the first refinement algorithm that is able to improve the quality of the original mesh. In this paper, the method has been applied to discretize the Brillouin zone of silicon for full band Monte Carlo device simulation. Densities of states for seven electron and hole bands of silicon are computed based on the new refined tetrahedral meshes.

Introduction

In 3D process and device simulation, creating a high quality mesh is critical for numerical stability and efficiency. Among all mesh generation methods, adaptive refinement is the most efficient way to improve simulation accuracy. Such an approach becomes important for discretization of the Brillouin zone of silicon for full band Monte Carlo simulation. In general, adaptive refinement of a tetrahedral mesh is difficult to accomplish without significantly degrading the mesh quality. Recently Leitner and Selberherr proposed a refinement method based on mixed-element decomposition [1]. This method limits the degradation of tetrahedral quality to a constant factor; however, it produces incompatible nodes which need special treatment during discretization.

Here we propose a new method called "Recursive Multi-Tree" (or "Recursive M-Tree") for adaptive refinement of a tetrahedral mesh. It can be shown that in the worst case, this method degrades the tetrahedral quality by a factor of 0.5; however, this corresponds to the refinement of an equilateral tetrahedron. For initial meshes of poor quality, this method actually improves the quality during the refinement process. This is important, as most initial tetrahedral meshes are usually far from perfect.

Recently, Bude and Smith have shown [2] that full band Monte Carlo device simulation can be accelerated up to 100 times using a tetrahedral instead of rectangular mesh for the discretization of the irreducible wedge of the Brillouin zone. We have used the Recursive M-Tree method for this application, and generated meshes for seven silicon bands. Densities of states have also been computed from tetrahedral meshes for the seven silicon bands.

Recursive M-Tree Algorithm

The Recursive M-Tree method starts on an initial coarse tetrahedral mesh. The algorithm first searches for the longest edge in the tetrahedron that needs refinement. Then, all tetrahedra that share that edge are searched for edges which are longer than the first edge. If the search come up empty, a node is inserted on the first edge. Otherwise, the refinement routine is recursively applied to the newly found (longer) edges, for which a search for even longer neighboring edges is then performed. This algorithm has two properties: 1) An edge is split only when it is the longest edge of all tetrahedra that share that edge. 2) An edge is split only because it does not satisfy the refinement criterion or there is another (shorter) edge in its neighborhood that needs to be refined. Property 1 assures that quality factor of the resultant tetrahedra are greater than 0.5. In most cases, however, this method improves the quality by splitting the longest edges. This is especially true for a poor quality initial tetrahedral mesh. Property 2 minimizes the number of nodes that are added. This decreases the number of nodes needed for the same refinement criterion when compared with other methods. For example, the minimum refinement in [1] is to divide a tetrahedron into 8 smaller tetrahedra. When an edge needs refinement we insert a node at the "center of mass" of all neighboring nodes on that edge. We found this improves the quality more than inserting a node at the middle of the edge. To demonstrate the quality improvement during refinement we use a long and narrow tetrahedron as an example (Fig. 1 inset). The refinement criteria is that the maximum edge length is shorter than 0.7. In this example the quality of the initial tetrahedra, defined as $Q \equiv 6\sqrt{2}V/h_{MAX}^3$ where V is volume and h_{MAX} is maximum edge length, is improved from 0.014 to 0.4. Note that a tetrahedron formed from a cube corner has a quality of 0.5. Also, this algorithm is computationally efficient. In another example (not shown here), 71.8 seconds CPU time were used to generated 1.1 million tetrahedra on an IBM/RISC6000 590 workstation.

Brillouin Zone Discretization

While full band Monte Carlo device simulation offers great physical detail about carrier transport in semiconductor devices, it is also very CPU intensive. CPU usage can be reduced by using an iso-energy surface aligned tetrahedral mesh [2] in the momentum space. This method can also be extended to a regular, non-aligned tetrahedral mesh by indexing the tetrahedra in lists sorted by energy. We have applied the recursive M-Tree algorithm to adaptively refine the irreducible wedge in momentum

space, producing a tetrahedral mesh that fills the domain, and represents the energy to the accuracy specified by the user. The error is defined as the difference between the original energy, computed from the quantum pseudopotential method, and the energy defined on the new tetrahedral mesh. The procedure is as follows: First, the irreducible wedge is divided into 3 large tetrahedra. Then, the refinement algorithm is applied with the refinement set to control the energy error such that the RMS error of the density of states is less than 5%. Meshes for seven silicon bands, comprising electrons and holes, have been generated. Compared with [2] this algorithm achieved better accuracy in representing carrier energy in momentum space with 40% less elements; at the same time, it is relatively easy to implement. Fig. 2 a and b show the meshes for the first bands of electrons and holes. Fig. 3 compares electron and hole density of states with those from a rectangular mesh [3]. Judging from the computational steps for the final momentum selection in full band Monte Carlo device simulation, our approach should yield similar CPU efficiency compared to that of Bude and Smith.

Conclusion

We have presented a novel method for adaptive refinement of tetrahedral meshes in 3D. Compared with existing methods, this algorithm is unique in improving the quality of the original mesh during refinement. Combining high efficiency as well as flexibility in the handling of various refinement criteria, this method provides a promising mesh generation tool for 3D process and device simulation. This method was applied to discretize the irreducible wedge for full band Monte Carlo device simulation. The densities of states of seven silicon bands were found to be in good agreement with those calculated from a rectangular mesh.

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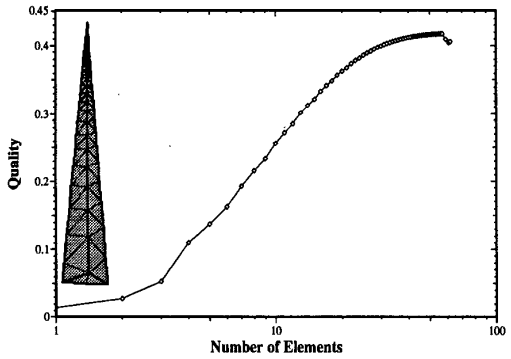

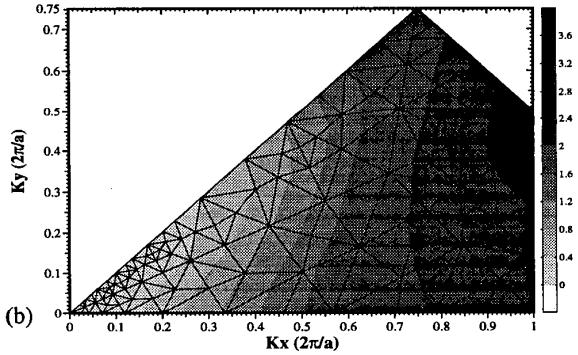

Fig. 1. Quality of tetrahedral mesh during refinement.

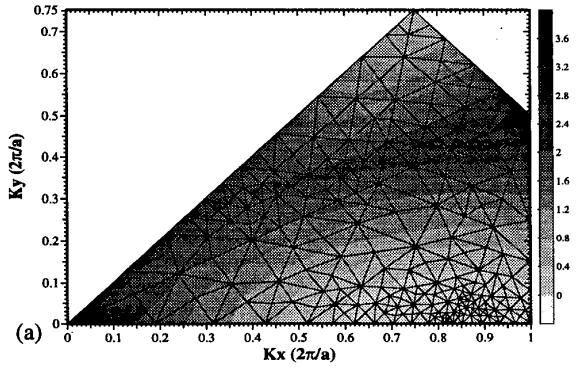

Fig. 2. z=0 projection of meshes for 1st conduction (a) and valence (b) band.

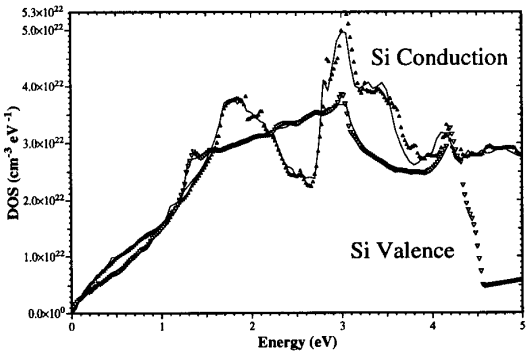

Fig.3. Comparison of DOS from the new tetrahedral meshes (symbols) and from rectangular mesh (lines).