Discretization of the Brillouin Zone by an Octree/Delaunay Method with Application to Full-Band Monte Carlo Transport Simulation

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Abstract

We present a fast octree/Delaunay method to generate a structured tetrahedral mesh in the Brillouin zone perfectly suited for the use with full-band Monte Carlo algorithms. The method permits local mesh refinements maintaining congruent tetrahedral face neighbors. Using Lagrange's remainder formula an estimate for the discretization error of the tetrahedral mesh elements is given. The method has been applied to investigate the influence of mesh refinements on full-band Monte Carlo transport simulations in silicon. In comparison with experimental data it is shown that high local mesh refinements are crucial to obtain accurate transport simulation results.

1. Introduction

Substantial efforts have been expended to develop physical models for full-band Monte Carlo (FBMC) transport simulations in Si [1-4]. However, even some of the most advanced models suffer from inaccuracies introduced by a too coarse discretization of the Brillouin zone (BZ) [2, 3]. Recently, FBMC simulations using tetrahedral meshes for the BZ discretization [5, 6, 3] have attracted a lot of interest. They are as fast as analytic band models [5] and they offer elegant solutions to several problems of the FBMC algorithm. Here, we propose a combined octree/Delaunay method to generate a tetrahedral mesh in the BZ perfectly suited for FBMC transport simulations. The method produces a structured mesh, i. e., the BZ is first subdivided into cubes and then the cubes are filled with tetrahedra. Unlike tensor-product grids [3, 6], which propagate unnecessary refinements along the coordinate axes, our refinement is locally restricted. Memory requirements are reduced and no tetrahedron is cut by BZ boundaries, which would otherwise require special treatment in the FBMC algorithm. Recently, Wang [7] presented a method for unstructured adaptive tetrahedral mesh refinement which starts from a coarse tetrahedral mesh. It has the disadvantage that the initial mesh which creates the best final one is not known, and that unwanted propagation from finer to coarser regions cannot be determined a priori.
The octree method has already been introduced in device and process simulation [8]. However, its combination with the point ordered Watson algorithm for the Delaunay tessellation [9, 10] proposed here has not yet been recognized in the field. By implementing the octree/Delaunay method in an FBMC programm we have investigated the influence of mesh refinements on transport simulations in Si. Excellent agreement with experimental data has been achieved, but only with highly refined meshes near the band edges.

2. Octree/Delaunay algorithm

The algorithm starts with the boundary description of the BZ geometry, or part of it, if symmetry can be used. It consists of two parts. The first (octree algorithm) creates the mesh points on cube corners according to a chosen density function. The second (Delaunay algorithm) fills each cube with tetrahedra assuring that tetrahedron faces on neighboring cube interfaces are congruent. The octree algorithm begins with a root cube containing the specified geometry. The edge length of this cube is compared with the density function. If the edge length is too large, the cube is divided into eight smaller cube children. The edge length of each child is again checked, and the algorithm stops when there is no need for further refinement. Cubes that do not have children are called complete cubes. Cubes can be inner cubes, outer cubes, or cut cubes with respect to the geometry boundaries. The next step is to traverse the tree to record for each complete, inner or cut cube whether mesh points from smaller cube neighbors or from cuts with boundaries lie on its faces or edges. A cube is called regular if this is not the case. Cube neighbors are not allowed to differ in their edge length by more than a factor of two. The Delaunay algorithm traverses the tree and fills each complete, inner or cut cube with tetrahedra. This Delaunay tessellation is done in two ways. If the cube is regular we use templates consisting of 5 tetrahedra (Fig. 3), or a mirrored set. Otherwise we use Watson's algorithm [10]. Introducing the mesh points in an ordered sequence we assure that tetrahedron faces of cube neighbors are congruent. In a last step the tetrahedron neighbor relationship needed for the full-band Monte Carlo algorithm is stored. The use of templates and the linear computation time dependence of the octree on the cube number makes the algorithm very fast.

3. Error analysis

The energy values at the mesh points (now corners of tetrahedra) are given by band-structure calculations. For Si we use nonlocal empirical pseudopotential calculations [11]. The discretization error at the mesh points is zero. Inside the tetrahedra we use a linear interpolation for the energy introducing an absolute discretization error which can be estimated for each tetrahedron by an analogue to Lagrange's remainder formula [12]: $e_{DIS} \leq 0.5 \cdot \hbar^2 / (M^* \cdot l^2_{MAX})$. Where l_{MAX} is the length of the longest edge of the tetrahedron, M^* is a positive lower bound for the effective mass, and $\hbar$ is Planck's constant divided by 2π. Unfortunately there seems to be no general lower bound of M^* for the whole Si band-structure [13], but around the band edges a value of $0.1 \cdot m_0$ will lead to a reasonable estimate. The results are shown in Table 1. Compared to the thermal energy of 38.8 meV at 300 K, and noting that the average carrier energy at a homogeneous field of 10^4 V/cm in Si is still less than 100 meV, it is obvious that a high refinement ($N_{DIV} > 64$) near the band edges is essential for meaningful simulations.

Refinement: N_{DIV}	16	20	32	64	128	256
maximum e_{DIS} [meV]	399	255	99.6	24.9	6.2	1.6

Table 1: Maximum discretization error of a tetrahedron with a longest edge of $l_{MAX} = 2^{1/2} \cdot l_{CUBE}$, $l_{CUBE} = 2\pi / (a_{Si} \cdot N_{DIV})$. $a_{Si} = 5.43$ Å is the silicon lattice constant.

4. Application to full-band Monte Carlo transport simulation

To investigate the influence of mesh refinements on transport simulations we consider three cases: Two of them use only regular cubes of one size, $l_{CUBE} = 2\pi / (a_{Si} \cdot N_{DIV})$, $N_{DIV} = 16$ or 32. $N_{DIV} = 16$ is a coarse grid. $N_{DIV} = 32$ is finer than the meshes in [2, 3] and requires an overall memory of 50 MBytes, which is already large for the use in

device simulation. The third case (variable discretization) uses the advantages of our octree/Delaunay method. Motivated by the error analysis, we keep the average relative error below 0.1% by varying N_{DIV} from 16 to 256, see Fig. 1. Only 25 MBytes are needed in this case. The influence of the three different meshes on the density of states (DOS) calculated from 8 Si bands is shown in Figs. 2, 3. It is obvious that near the band edges only the variable discretization gives the correct square root dependence of the DOS.

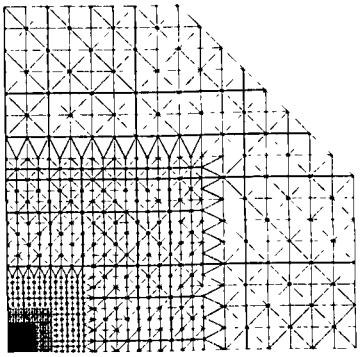

Figure 1: BZ cut ($k_z = 0$, $0 \le k_x, k_y \le 2\pi / a_{Si}$) of the tetrahedral mesh used in the case of variable discretization for the first valence band. N_{DIV} varies from 16 to 256.

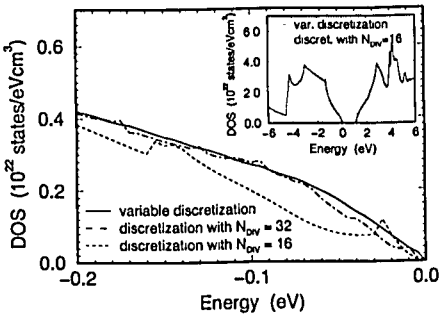

Figure 2: Density of states near the band edge of the valence band for different mesh refinements. Inset: DOS on a larger scale.

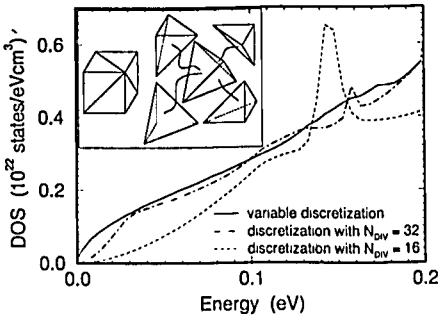

Figure 3: Density of states near the band edge of the conduction band for different mesh refinements. Note that the conduction band minimum has been shifted to the origin by the bandgap energy. Inset: Set of 5 tetrahedra building a regular cube.

Transport has been calculated with an FBMC model similar to [5], but using energy dependent optical and elastic acoustic phonon scattering rates. Table 2 shows the results for the low-field hole mobility. Only the mobility obtained with the variable discretization agrees with the experiment within the FBMC statistical error. The $N_{DIV} = 32$ value deviates already by 50%. Surprisingly, the high-field results of the hole drift velocity for $N_{DIV} = 32$ (Fig. 4) show considerable deviations from the experimental values up to fields of 10^4 V/cm. In contrast, excellent agreement is achieved with the variable discretization. FBMC simulations of electron drift velocities, not presented here, yield similarly strong discretization effects whereas it is important to notice that the average carrier energy depends only weakly on the discretization. In conclusion, the proposed octree/Delaunay method promises to provide an excellent basis for future highly accurate and efficient FBMC device simulations.

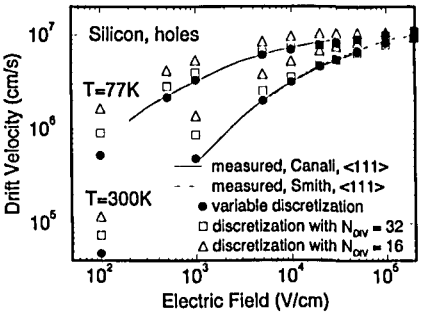

Figure 4: Hole drift velocity versus field. The experimental data is from [14] (solid line), and [15] (dot-dashed line). FBMC transport parameters: $D_{AC} = 3.65$ eV, $v_S = 6540$ m/s, $D_{OP} = 9.5 \cdot 10^{10}$ eV/m, $\hbar\omega_{OP} = 63$ meV. The FBMC statistical error is $< 5\%$ except for the values at 10^2 V/cm given in Table 2. The confidence level is 99.7%.

$\mu_{Si,hole}$ [cm^2/Vs]	Exp. [16]	Var. Discret.	$N_{DIV} = 32$	$N_{DIV} = 16$
	505	478 ± 48	750 ± 36	1175 ± 72

Table 2: Low-field hole mobilities, calculated from $\mu = v_d / E$. $E = 10^2$ V/cm, $T = 300$ K.

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