A Computationally Efficient Model for Three-dimensional Monte Carlo Simulation of Ion Implantation into Complex Structures

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Abstract

A new three-dimensional Monte Carlo simulator has been developed based on UT-MARLOWE. Unbalanced Octree algorithm was used for spatial decomposition. A new trajectory replication scheme was developed and implemented to enhance computational efficiency. More than two orders of magnitude savings on CPU time have been achieved.

Introduction

Monte Carlo simulations of ion implantation into three-dimensional complex structures typically lead to severe challenges in term of computational efficiency. In order to obtain the same level of statistical significance for the overall structure, the number of incident ions at each specific grid cell must be kept approximately at the same level as for 1-D and 2-D simulations. *Approximately, for each additional dimension, the required number of ions for Monte-Carlo simulation should increase by about two orders of magnitude.*

New 3-D Trajectory Replication Scheme

Although not adequate to be applied to three-dimensional simulation directly, lateral trajectory replication scheme [1] provides a good insight into the problem. The key is to cleverly reuse the physically-computed trajectories for similar topography.

The lateral trajectory replication scheme is shown in Fig. 1. It starts by physically calculating all the required scattering events and the stopping mechanisms experienced by one particular ion until it stops. The algorithm then introduces an offset and replicates the model trajectory at the new incident position. At the same time, replication error is examined according to two factors: whether the material in the model trajectory matches that in the target trajectory and whether the damage level is comparable between them.

A schematic of how the new replication scheme proceeds is shown in Figure 2. The implant window is divided into small rectangles or squares. The first ion is set to implant into the left bottom corner segment and the trajectory is physically-

computed and recorded. The initial relative position within the segment is determined randomly. Replication then proceeds up and to the right of the original trajectory. When an error occurs, replication stops, the trajectory is recomputed and the model trajectory is replaced with the newly calculated one. Thus, the simulator is able to *intelligently* reuse physically-calculated trajectories in two directions. Since the CPU time required to replicate is much less than the time required for the actual physical computation, large savings are expected with the application of the new replication scheme without sacrificing accuracy, as shown in Figures 3, 4.

Structure Decomposition

As the ions are propagating through the structure, the determination of the material type is crucial and could be very CPU time consuming. An unbalanced Octree decomposition scheme is adopted in this new simulator. Similar to the Quadtree decomposition scheme [1,2], Octree also recursively subdivides space until the desired resolution is reached. Octree structure offers two major advantages over other structured and unstructured meshes. First, it simplifies the structure since the resulting grid is coarse where the material is uniform, and fine near the material interfaces. Secondly, the tree data structure makes the tracking more efficient (proportional to logN, instead of N), and reduces the zoning time accordingly.

Model Verification

The physical models used by the new simulator are based on UT-MARLOWE and have been extensively verified.

In this simulator, two models have been provided to simulate ion implantation into poly-silicon. The first model uses amorphous silicon to represent poly-silicon, and the second one, or the worst case channeling scenario, uses a deterministic Monte Carlo model and simulates implant into a (110) wafer. Implantation into a (100) wafer with both tilt angle and rotation angle set to 45 degrees is equivalent to implantation into (110) wafer with both tilt angle and rotation angle set to 0 degrees. Therefore, we can compare the converted 1-D profile with SIMS data for the same implant condition into a (100) wafer with both tilt and rotation set to 45 degrees. As shown in Figure 5, for As 50keV implantation, the SIMS data and the converted simulation results match very well. In addition, As channeling through a three-layered structure, polysilicon, gate oxide and crystalline silicon was studied as shown in Figure 6.

References

1. B. Obradovic, etc, IEDM 1998 Technical Digest, 513.
2. G. F. Carey, etc. "Computer Simulation of Semiconductor Processes and Devices-- Mathematical and Numerical Aspects", John Wiley and Sons, 1996.

Figure 1. Side view of the replication algorithm proceeding from left to right. Light trajectories are physically computed, gray ones show where replication error occurs, and black ones are replicated trajectory.

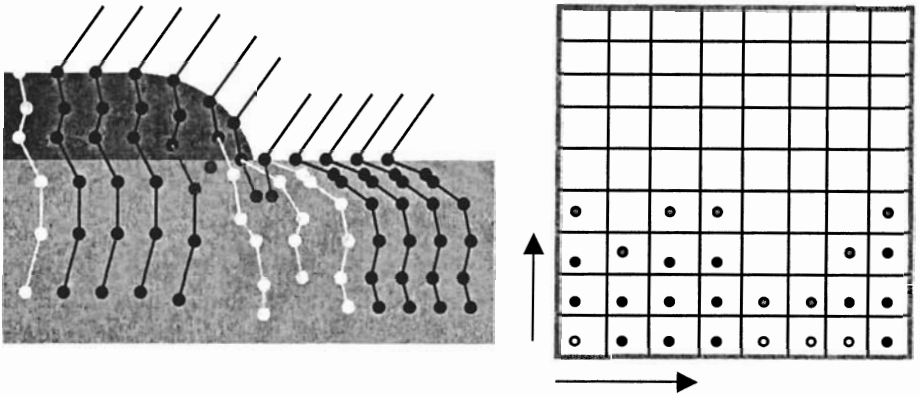

Figure 2. Top view of the simulation domain illustrating the replication algorithm. Hollow circles are physically computed, gray ones show that replication errors are encountered and trajectories are therefore physically computed, and black ones are replicated. Replication starts from the left bottom corner and proceeds up and to the right of the original trajectory.

Figure 3 (a). Simple trench topography for replication scheme demonstration. The length of the whole volume is 800 lattice constants. Depth is 700 lattice constants.

Figure 3 (b). Simulating boron 5keV implant into structure shown in Figure 3(a), tilt-7°, rotation-30°, dose-$1\times10^{14}cm^{-2}$. CPU time is 72 minutes using 5,000,000 ions. The iso-concentration contours range from $1\times10^{15}cm^{-3}$ to $1\times10^{17}cm^{-3}$. Estimated CPU time *without replication* is over 20 hours.

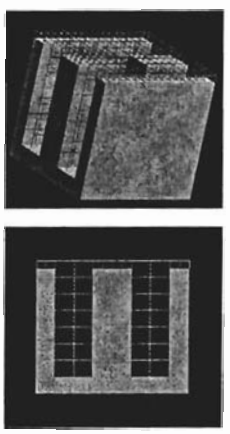

Fig. 2

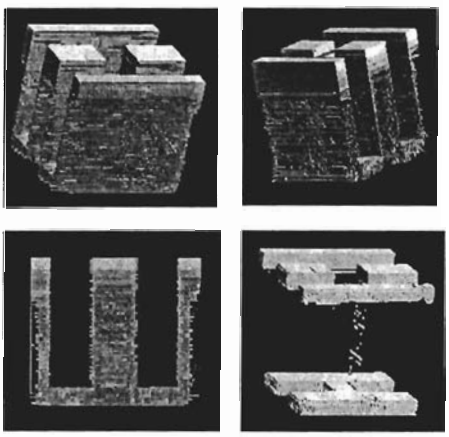

Fig. 3

Figure 4 (a). Source/Drain structure with shallow trench isolation. Side length is 600 lattice constants.

Figure 4 (b). Simulating arsenic 15 keV implant into structure show in Figure 4(a), tilt-0°, rotation- 0°, dose $1\times10^{13}cm^{-2}$. CPU time is 88 minutes, using 5,000,000 simulated ions. The iso-concentration contours range from $1\times10^{16}cm^{-3}$ to $1\times10^{19}cm^{-3}$. Estimated CPU time *without replication* is over 20 hours.

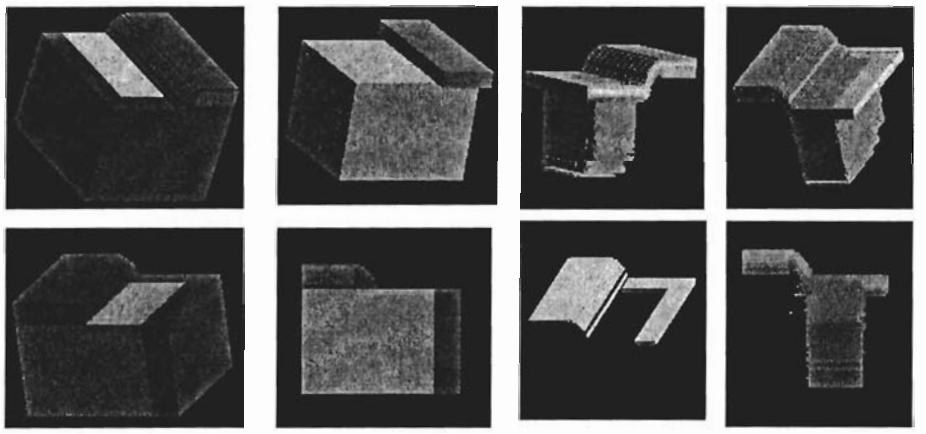

Figure 5. Profiles of a 50keV As on-axis implant into a (110) Si wafer with a dose of $2\times10^{12}cm^{-2}$ to simulate the worst case channeling scenario of an implant into poly-silicon.

Figure 6. Profiles of As on-axis implant into a three-layered structure (100nm polysilicon, 2.7nm gate oxide and 700nm crystalline silicon) at 1, 3, 8, 15, and 30 keV with a dose of $1\times10^{15}cm^{-2}$

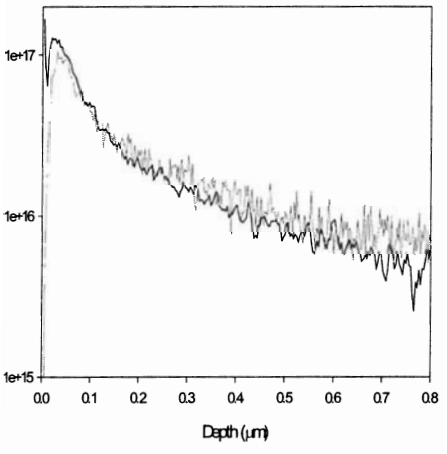

Fig. 5

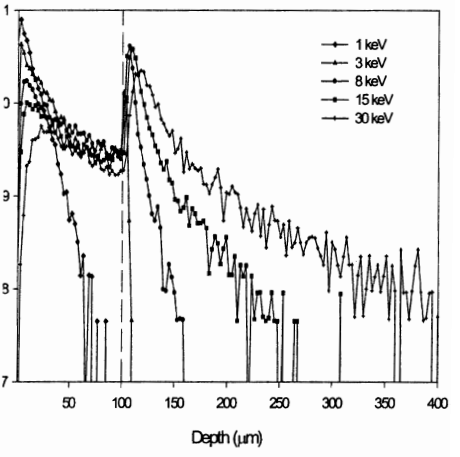

Fig. 6