A Moving Mesh Method for Device Simulation

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Abstract—A moving mesh method for semiconductor device simulation is developed which effectively compromises accuracies without increasing mesh number. In this method, mesh positions are shifted referring to the solution of the previous bias condition, or to the Newton corrections. The method is applied to solve PN-junctions and MOSFETs. The method provides an effective way to cover the changes of carrier distributions depending on bias conditions. The algorithm is simple and effective, and can be widely used.

Keywords—semiconductor device simulation; mesh; algorithm;

I. INTRODUCTION

Recent market expansion of power devices makes device simulations more important [1]. In power devices, depletion regions extend widely, since large biases are applied to low concentration semiconductor substrates. Because the depletion regions are changed drastically depending on device structures, doping concentrations and applied biases, it is hard for simulation users to know how to set mesh points before the simulation. Historically, such problems are tackled by re-mesh techniques which use new additional mesh points to cover the expansion of the critical regions [2]. This causes the increase of CPU time instead. From the view point of device simulation users, the carrier profiles steeply change around depletion region edges in most of the cases. And the depletion region edges move depending on the bias conditions. Therefore such steep positions may move gradually with increasing or decreasing the applied biases. This paper challenges such problems by simply moving the meshes to cover the widely changed physical distributions, referring to the solutions of the previous bias conditions.

II. ALGORITHM

In semiconductor device simulations, it is very important to set enough mesh points where physical quantities are steeply changed. Especially carrier concentrations are the important variables whose values change many orders of magnitude. For device simulation, accuracy depends on the number of mesh points where carrier concentrations change steeply. Even though the simulation users have common knowledge about semiconductor device physics, it is very hard to predict such physically steep positions before simulations, especially for 2D or 3D cases. Furthermore, these physically steep positions move depending on bias conditions. Typical examples of such positions are depletion region edges of PN junctions which move widely depending on the bias voltages, especially in high-voltage devices.

The basic idea of the present work is shown in Fig. 1. In an N+/P junction the depletion region edge moves depending on the applied reverse bias conditions. Carrier concentration profiles are steeply changed at these depletion edges. Therefore, in order to keep the simulation accuracies, the minute mesh points should be at these depletion edge positions, which move gradually depending on the reverse bias conditions. On the other hand, in the middle of the depletion regions, the carrier concentrations are very low and not so many mesh points are required there. Here comes a simple idea to move mesh points towards the depletion edges. To enable such mesh controls, physical quantities solved at a bias condition are used to search critical positions where more mesh points are required.

Fig. 1. A basic idea of the present work. The depletion edge of an N+/P junction moves depending on the bias conditions. This means that the minute meshes should also be moved depending on the bias conditions.

The basic flow chart of the present method is schematically shown in Fig. 2. The device structure including material, doping profiles, and mesh points are saved initially, as the reference of the following re-meshing. In this algorithm, it is very important to determine the mesh points which should not be moved corresponding to material boundaries and electrodes. These points are fixed and not moved throughout the simulation.
Fig. 2. The basic algorithm of the present moving mesh approach. Mesh points are evaluated using the previous bias step, and movements of the meshes are determined. Impurity profiles are re-mapped by interpolations.

After solving the first bias condition using the initial mesh, the directions and the distances of the mesh points to be moved are determined by evaluating distributions of physical quantities or their Newton corrections. These evaluations are the critical key points to engage the efficiency of the present method. The scheme of these evaluations can be modified depending on the target devices, bias conditions, and simulation objectives.

A basic idea of these evaluations and mesh movements is schematically shown in Fig. 3. Consider the mesh point ‘i’, the previous Newton corrections ($\Delta n + \Delta p$) of both sides ‘i-1’ and ‘i+1’ are compared. Such parameters to be compared can also be second derivative of the carrier profiles. In this figure, the correction of the ‘i-1’ point is larger. In this case, it is required to get more minute mesh around ‘i-1’ than around ‘i+1’. Therefore the mesh point ‘i’ is moved toward ‘i-1’ direction. Such evaluations and movements are applied to all mesh points excepting the fixed mesh points determined in the second step of the flow chart.

After moving the meshes, the impurity profiles are re-mapped by interpolation scheme referring to the saved initial device structure. This ensures the stability of the device structure even after many re-mesh events. It is optional to solve the same bias condition after the re-mesh, before proceeding to the next bias condition. Although there may be several variations of these algorithms, the key points of the present approach are included in Fig. 2.

III. APPLICATIONS

Three types of applications are demonstrated to show the efficiency of the present moving mesh method. 1D, 2D N+/P junctions, and 2D MOSFETs which are typical targets of semiconductor device simulations.

A. 1D PN-junctions

The method is applied to a simple 1-dimensional N+/P junction analysis. The initial mesh is manually created with the common ratio intervals. The key of the method is how to move the mesh points. Authors have tried several criteria, and found the second derivatives of the logarithms of net carrier concentrations weighted by mesh sizes are successful criteria. Another key is that mesh sizes are restricted between the minimum and the maximum mesh sizes specified by users. Fig. 4 shows the depth profile of the electron and the hole concentration of the N+/P junction, for reverse biases of $5V$ and $30V$. For both bias conditions, number of the mesh points is same. The mesh points move corresponding to the depletion region width.

### Fig. 4. Mesh points of an N+/P junction which move depending on the depletion region edge by the criteria of second derivatives of carrier concentrations.

The other successful criteria use Newton corrections of carrier concentrations as the evaluation parameters to find the critical positions. Fig. 5 shows mesh points with carriers and electro-static potentials for the reverse biases of $5V$ and $50V$. In Fig. 6, I-V characteristics of with and without the present moving mesh method are compared. Without the moving mesh, the I-V curve contains abnormal step-wise fluctuations, which
are typical problems caused when the depletion edge moves over the one mesh to the next rough mesh.

It is worth mentioning that the smooth $I-V$ curve is obtained even with some rough mesh sizes observed around 2µm-depth in Fig. 5. From this fact, the possibility of the present method to save CPU resources of device simulation is optimistic, because the present method has an ability to enhance simulation accuracy automatically. In other words, to investigate the better criteria of the moving mesh method is to optimize mesh positions for better accuracies which is a very fundamental issue of the semiconductor device simulation.

It is important to comment on the difference of $I-V$ curves in Fig. 6. The red curve without the moving mesh method has not only a numerical instability, but also has errors of absolute values of the currents. This comes from the fact that small numbers of mesh points are used for the calculations of both curves. If the numbers of the mesh points for the red curve is increased, the $I-V$ curve converges into the blue curve. In other words, the present method provides the better accuracy for the same number of mesh points.

**B. 2D PN-junctions**

Fig. 7 shows an example of a 2D N+/P junction case. Meshes are moved both vertical and horizontal directions to cover the expansion of the depletion region. Both the second derivative of carrier concentrations, and the relative Newton corrections of carriers are successful criteria to obtain directions for meshes to be moved, and Fig. 7 is the case of the second derivative criteria. When the larger reverse bias voltage is applied to the junction, depletion region extends drastically as hole concentration depletes in the case of 5-V. In the present method, the simulator evaluates the carrier Newton corrections in order to adjust the positions of mesh points automatically.

It is clear that this method is more effective for power devices which use large depletion regions to avoid the breakdown. It is also clear from this figure that the present method is more effective for multi-dimensional cases, such as 3-dimensional simulations of power devices.

Fig. 7. An example of the present method applied to a 2D N+/P junction.

Fig. 8 shows another example of a 2D N+/P junction up to the bias condition of 50V, using the carrier Newton corrections criteria for mesh evaluations. Hole concentrations are shown by a color map, and wide hole depletion region is clearly observed which is efficiently covered by minute mesh points moved by the present method. In Fig. 9, $I-V$ characteristics obtained with and without the present method using the same number of mesh points are compared. In the red $I-V$ curve without the moving mesh, the same type of step-wise instability as in Fig. 6 are clearly observed again.

The $I-V$ curve instability in Fig. 9 comes from the errors of generation currents of the Shockley-Read-Hall mechanism occurred in the depletion region. Because of rough meshes at depletion edges, generation rates at each mesh volumes differ between neighbor mesh points as shown in Fig.10. This is the main reason of the step-wise instability of the $I-V$ curve obtained by rough mesh device simulations.

Fig. 8. An example of the present method applied to a 2D N+/P junction up to the bias condition of 50V.

The $I-V$ curve instability in Fig. 9 comes from the errors of generation currents of the Shockley-Read-Hall mechanism occurred in the depletion region. Because of rough meshes at depletion edges, generation rates at each mesh volumes differ between neighbor mesh points as shown in Fig. 10. This is the main reason of the step-wise instability of the $I-V$ curve obtained by rough mesh device simulations.
C. 2D MOSFETs

Fig. 10 shows an example of a 2D nMOSFET. Meshes are moved to cover the depletion region which is affected by the gate biases. Thus for such complicated cases, the present method provides a way for simulation users to avoid careful management of meshes by predicting the results in their brains.

Fig. 11. An example of the present method applied to a 2D MOSFET case.

IV. SUMMARY

A moving mesh method for semiconductor device simulation is presented, which enables the automatic adjustment of mesh positions to cover important regions to be solved. Second derivatives of the logarithm of net carriers, and Newton corrections of net carriers are successful evaluation criteria of the mesh movement. The scheme is applied to PN-junctions and MOSFETs, and is found to be an effective tool for device simulation users to avoid careful mesh considerations before applying bias conditions.

REFERENCES
