3D TCAD at TU Vienna

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Abstract

This paper gives an overview about our research on three-dimensional process simulation. Today's activities are worldwide still suffering from a lack of appropriate geometric modeling, robust gridding, accurate and verifiable physical models as well as computationally efficient numerical algorithms. Possible solutions to some of these problems are demonstrated on the basis of our three-dimensional process simulation tools.

1. Introduction

The development of today's semiconductor devices often requires to investigate three-dimensional problems, where in many cases numerical simulation delivers useful information. For the reliability of such hints the accuracy of the simulation results is crucial. The effects occurring at intrinsic three-dimensional topologies, like corners etc., are gaining importance with shrinking device dimensions. Thus, consideration of the third dimension within the simulation is a must for both process and device simulation.

In contrast to three-dimensional device simulators which are available from universities as well as from commercial sources, the situation in process simulation is quite different: Today it is not possible to perform a complete three-dimensional simulation of a whole process. Impressive work on topography simulation resulted in excellent programs for surface evolution during etching and deposition processes [1] [2]. An engineering workstation is sufficient for this kind of simulations. Also programs for ion implantation based on Monte Carlo methods are available [3] [4] [5]. Where the first versions consumed CPU-times beyond one week (on an HP9000-735), recent developments allow to compute realistic three-dimensional results over night in the amorphous mode, respectively one day for the crystalline mode. Despite these encouraging results, simulation of a whole process fails on missing diffusion and oxidation simulators. Although some three-dimensional simulators have already been presented [6] [7], the complex structures of realistic devices cannot be handled by them because of the lacking grid flexibility.

Therefore development of fully flexible three-dimensional diffusion and oxidation simulators is highly recommended. However, the problems involved are quite complex. Modern devices have more or less arbitrary geometries which are difficult to handle, and the simulation of thermal activated processes requires the solution of coupled, nonlinear partial differential equation systems. This just can be achieved efficiently
by use of adaptive gridding techniques as well as highly efficient algebraic methods. Additional challenges lie in the simulation of thermal oxidation, where the diffusion equations and the mechanical equation have to be taken into account. The resulting changes of the geometry reveal high demands to the gridding unit, and additionally the stiff mechanical equations expense the solution of the linear systems. This extremely high complexity within one application has scared of many researchers from tackling the problem.

Besides the numerical and geometrical problems, the quantization of the parameters required by the differential equations accounts for a great deal of controversy. Even for one-dimensional diffusion processes, where the profiles can be measured with satisfying accuracy, the range of the proposed diffusivities is quite large. The situation is even worse for the properties of the point defects: Since it is impossible to measure point defect distributions directly, these are usually quantified due to their effects on the dopant distribution. E.g., the initial distribution is chosen, in order to reach the desired influence on dopant diffusion using a certain set of coupling coefficients. These coupling coefficients have to be determined by calibration of the coefficients, which in turn is influenced by the initial condition. Thus, the missing orthogonality allows to produce almost any result.

Furthermore, it has been pointed out [8], that the lack of multi-dimensional measurement techniques inhibits the calibration of corresponding multi-dimensional simulation tools. On the other hand process simulation seems to be the only possibility to obtain multi-dimensional profiles, because of the insufficient measurement techniques. One may speculate that once we will have reliable one-dimensional physical models, their usage within multi-dimensional simulators will allow to predict doping profiles much more accurately than any measurement technique.

Finally, achieving a complete simulation of a three-dimensional process-flow demands highest flexibility in data management. Data exchanging between different simulators using different data representation forms for geometries (e.g. cellular based, octree based or polygonal based) and profiles stored at different grid types account for a large additional effort which is necessary to couple different simulators effectively. As an example, the generation of a tetrahedral grid for a device geometry computed by a topography simulator such as [1] needs first to convert the cellular based geometry to a polygonal based one. Then the polygonal surface has to be adapted in order to fulfill some conformity conditions and grid points within the solids have to be computed before the tetrahedrization algorithm can be applied. Furthermore, optimization of the grid in terms of element quality and minimum node count requires some kind of optimization loops. All those steps suffer on the enormous amount of data and the structural complexity to be dealt with.

Our work regarding the three-dimensional process simulation resulted in several process simulation modules: In Section 2 we present our simulator for surface evolution and the coupling with physical models for etching and deposition processes. Section 3 deals with the ion implantation module and recent improvements there. In Section 4 we present our module for diffusion processes, and finally, Section 5 contains an outlook on our attempts to tackle three-dimensional oxidation simulation.