Three-Dimensional Simulation of Ion Implantation

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With shrinking dimensions and growing complexity of advanced ULSI devices three-dimensional effects are becoming more and more important for their development and optimization. For this reason, within the project PROMPT a multidimensional process simulation software capable to provide appropriate input to three-dimensional device simulation has been developed by a European consortium [1-4]. The PROMPT software compiles the geometry and the dopant profiles of the device from the results of existing one- and two-dimensional process simulators and three-dimensional modules newly developed. Within this presentation, the capabilities of the three-dimensional ion implantation module developed at FhG-IIS-B within PROMPT are being outlined.

Critical for three-dimensional simulation of ion implantation are both the use of advanced physical models to appropriately describe effects like tilt and rotation of the ion beam, channeling, and implantation through multilayer masks, and the need to limit the computation time required to acceptable values. To meet these two targets, an approach has been developed at FhG-IIS-B which starts from a key variable of advanced multilayer models, namely the effective thickness of the material on top of the point in question, calculated parallel to the ion beam. This value t_{eff} is calculated according to

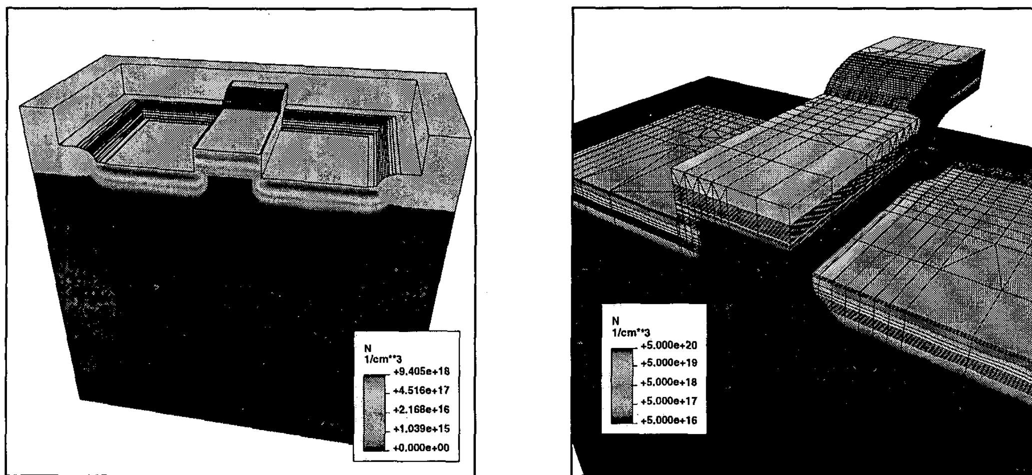
$$t_{eff} = \sum_{i=1}^{n} \frac{t_i}{R_{p,i}}$$

Here, t_i is the length of that part of the ion beam passing through the point in question which lies in layer i, and $R_{p,i}$ is the projected range of the implanted ion in the material of that layer. In order to calculate the implanted dopant concentration at a certain point, advanced multilayer models developed at the institute (e.g. [5],[6]) only need the value t_{eff}, and partly also similar expressions with weighting factors different from $1/R_{p,i}$, at each point of the numerical convolution to be calculated in a multidimensional model. In terms of physical parameters, a complete set of vertical, lateral, and mixed range moments is required [7]. Whereas for amorphous targets these parameters are available from Boltzmann transport calculations [8], the influence of ion beam orientation with respect to the crystalline structure has been treated by extracting the range parameters required from crystalline Monte-Carlo simulation [9]. The geometrical implications are directly predicted by the three-dimensional simulation module.

The analytical simulation of ion implantation includes the calculation of a convolution integral for each mesh point. For this integral, advanced vertical and lateral models require the calculation of t_{eff} at each convolution point. Simple arithmetics shows that the standard approach which determines all intersections between the line parallel to the ion beam passing through the convolution point and the in general nonplanar surfaces of all masking layers would require huge computation times of about one day, because generally a fine resolution of the convolution integral is needed if it is not automatically adapted to the changes of the topography, e.g. at mask corners nearly parallel to the beam direction. Therefore, a new approach has been developed and implemented in three dimensions. In this approach, a separation of the necessary topography treatment and of the calculation of the dopant concentrations is achieved by a topography projection algorithm: All surface triangles are projected to a reference plane which is perpendicular to the ion beam direction, and the distances d between the vertices of the original surface triangles and the reference plane are stored as an attribute of the projected triangles. In order to correctly treat overhanging structures, the sign of d is set equal to the sign of the scalar product between the ion beam direction and the surface triangle normal oriented into the layer. Furthermore, the value is scaled by the projected range $R_{p,i}$ of that layer. For each point where the implanted dopant concentration is to be calculated it is checked in which projected triangles the projection of the point lies. The values for d for these triangles are then used to calculated t_{eff} for the mesh point in question. Because the contribution of each triangle to t_{eff} behaves linearly within the triangle, the algorithm outlined calculated t_{eff} without any interpolation errors. Furthermore, it also allows for easy adaptation of the integration mesh used in the lateral convolution. In con-

sequence, the numerical error is controlled, and the numerical effort needed is no longer proportional to the product of the number of surface triangles, mesh points, and convolution points per mesh point, but is only proportional to the number of mesh points times the number of convolution points, and hardly depending on the overall number of surface triangles.

The algorithm outlined above has been implemented in three dimensions, and has been successfully evaluated using own and industrially specified benchmarks. Fig. 1 shows the 3D simulation of ion implantation during the fabrication of a CMOS structure, following a process flow specified by the PROMPT partner GPS. The 3D ion implantation module has been interfaced with the mesh generator OMEGA [10] of ETH Zurich, in this way allowing for automatic mesh adaptation during ion implantation simulation. In Fig. 2, tilt and rotation of the boron ion beam have been changed to 45° and 27°, respectively. Parameters suitable for the implantation into crystalline silicon at an energy of 20 keV under these conditions were used. For the figure, the oxide and resist layers have been removed after the implantation step, and the mesh is also shown in the figure. Due to tilt and rotation, the polysilicion gate running across the field oxide leads to a strong 3D effect in the implanted dopant concentration, as shown. This shadowing effect which due to geometrical reasons only occurs at one side of the poly gate cannot be simulated using existing two-dimensional tools. It modifies the effective channel width and length and should in this way also influence electrical behavior. Computation time for this example was 27 minutes for the calculation of the implanted dopant concentrations on about 83 000 mesh points, without the time needed by OMEGA for mesh generation.



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