EFFICIENT MULTIDIMENSIONAL SIMULATION OF ION IMPLANTATION INTO MULTILAYER STRUCTURES

J. Lorenz, R.J. Wierzbicki¹ Fraunhofer-Arbeitsgruppe fuer Integrierte Schaltungen Artilleriestrasse 12, 8520 Erlangen, Germany

> ¹Lehrstuhl für Elektronische Bauelemente Cauerstrasse 6, 8520 Erlangen, Germany

For the three-dimensional simulation of ion implantation into multilayer structures, the computing times of straight-forward analytical approaches increase in comparison with two-dimensional simulations. Therefore, the advantage of such approaches compared with Monte-Carlo simulations in terms of computing times decrease if in the Monte-Carlo simulation the number of particles traced is reduced by efficient multiple use of particle trajectories as described by Hobler [1]. In this paper, a novel approach is described which drastically reduces the numerical effort needed for the calculation of analytical expressions for ion implantation into two- or three-dimensional multilayer structures. Model improvements are discussed.

The main problem in the multi-dimensional analytical simulation of ion implantation is caused by the convolutions needed to describe the lateral implantation profiles. These convolutions involve products of vertical multilayer distributions, e.g. using the Improved Numerical Range Scaling model [2], with lateral Pearson distributions [3]. The vertical distribution depends on the thicknesses of the masking layers which may vary in lateral direction, see Fig. 1. Furthermore, also the lateral distribution depends on the masking layers due to depth-dependent lateral range straggling [4] and kurtosis. Thicknesses of masking layers may change discontinuously in lateral direction, e.g. at mask edges. In order to avoid large errors with the calculation of the lateral convolution, many convolution points are necessary at least below mask edges. For the calculation of the thicknesses of masking layers along the direction of ion implantation above a point of interest, it is generally necessary to





Implantation beam for 7° tilt near a nonideal mask edge. Projected boundary points along horizontal mesh line are also shown.

check for the intersection of the implantation beam with a large number of polygon segments or plains which confine the masking layers, see Fig. 1. This means that in case of a straight-forward calculation of the lateral convolutions a large numerical effort is necessary especially for three-dimensional simulations.

In the noval approach, the profile implanted is calculated for the points of an adaptive mesh which is controlled by the ion implantation itself. Dopant concentration values are calculated for the topmost horizontal line (2-d) or plain (3-d) of a quadtree- or octtree mesh. For this line or plain, also the projections of important boundary points which describe the wafer topography are calculated, together with the distances to the layer surface and/or the thicknesses of covering layers along the implantation beam which is in general tilted. This procedure is then continued for the next line or plain in downward direction. Furthermore, the lateral distance of mesh points for the next line or plain is estimated based on the concentration values of the actual line, and the vertical position of the next mesh line or plain is controlled based on the values on the actual and the preceeding line or plain. This results in a 2-d or 3-d adaptive mesh

which is generated simultaneoulsly with the implanted profile. Because the projections of the boundary points are known on the mesh line or plain in question, the effective thickness of the target material above the point where the concentration is being calculated can be obtained without discretization error from linear interpolation, and, for the same reason, the lateral Pearson distributions needed in the convolution can be efficiently calculated from logarithmic interpolation between the projected boundary points with good control of interpolation error. This algorithm allows the efficient implementation of advanced models for residual channeling and depth-dependent lateral spread and kurtosis, which are in general depending on the thickness of all layers above the point in question. In Fig. 2, a simulation of the implantation of 60 keV boron using a refined model for the depth-dependent lateral spread is compared with Monte-Carlo simulations using TRIM [5]. The excellent agreement between the result from the analytical model and from the Monte-Carlo simulation are due to the use of a parabolic dependence of the lateral spread on depth above the profile maximum and an exponential dependence below the maximum. The range parameters used in the lateral model where taken from tables calculated with the Boltzmann-transport program RAMM [4].



Fig. 2: Comparison between simulation using the refined model for the depth-dependent lateral spread and Monte-Carlo simulation for implantation of boron with an energy of 60 keV: a) lateral range straggling versus depth, b) 2d profile near mask edge.

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