Monte Carlo Simulation of Ion Implantation into Two- and Three-Dimensional Structures

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Until now, Monte Carlo simulation of ion implantation into 3D-structures has been prohibited by the huge amount of CPU-time required. In this paper a method is presented which makes 3D-simulations with simple geometries feasible as well as 2D-simulations with arbitrary geometries. The method is applied to the sidewall doping of trenches.

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Until now, Monte Carlo simulation of ion implantation into 3D-structures has been prohibited by the huge amount of computer time required. Also 2D-simulations have been restricted to simple geometries such as linear mask edges or rectangular trenches. The reasons are:

(i) Resolving additional details, e. g. in the third dimension, requires a larger number of simulated particles.

(ii) For complex geometries the time determining part of the program is the detection of particles crossing surfaces and/or interfaces.

In this work we present a method which reduces these problems substantially. A target consisting of only one material is assumed. This, however, is not a severe restriction for Si technology: Even in the case of SiO_2- or Si_3N_4-layers, the stopping of ions in these materials is similar to the case of Si. The main features of the method are:

(i) Each "physical" ion trajectory is used several times to determine the history of ions entering the target at different positions. Thus physical quantities like scattering angles need only be calculated once for a set of trajectories. A reasonable value for the distance between incidence points of ions within the same set is the lateral standard deviation of the corresponding point response.

(ii) A grid is used to reduce the time required to detect ions crossing surfaces. Every grid element is assigned the minimum distance between any point inside the element and the surface. Thus, knowing that an ion is inside grid element i, that grid element i has a minimum distance d from the surface, and that the free flight path is l, one can conclude that the ion may not cross the surface within the next d/l free flight paths. (To check whether an ion crosses the surface is done by intersecting the free flight path with all lines of the surface.)

With these two features a reduction of CPU-times by factors of 10 to 100, depending on the complexity of the geometry, could be achieved.

The new method is applied to the sidewall doping of trenches by ion implantation. We have made comparisons (1) between an ideal, rectangular trench and a trench with surface roughness, and (2) between a trench with infinite width (in the "third" dimension) and a trench with quadratic cross section. We have also checked feature (i) of our method by comparing the results of a 2D-simulation with those of a conventional simulation. No difference could be detected, neither in concentration values nor in statistical fluctuations.

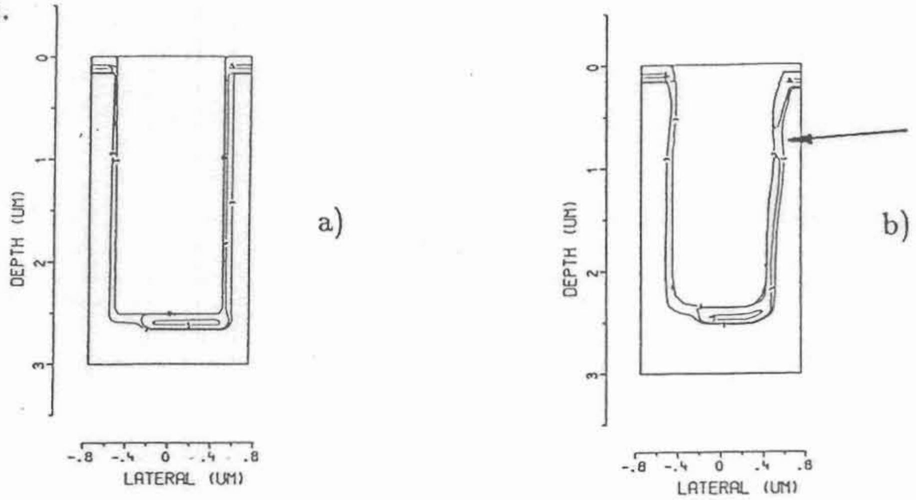

Fig.1: Boron implantation (25 keV, tilt angle 7°) into an ideal trench (a) and a trench with surface roughness (b). The surface roughness causes an inhomogeneity of the doping at the sunny side (see arrow).

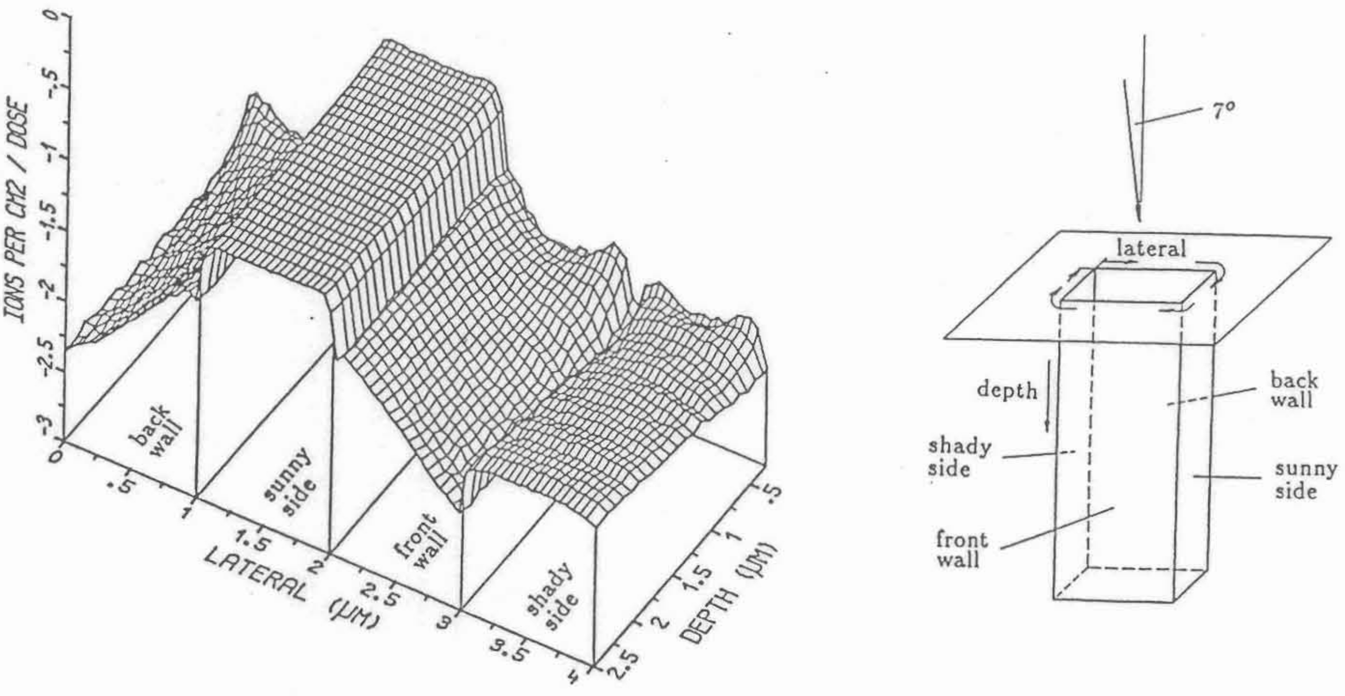

Fig.2: Boron implantation (25 keV) into a trench with quadratic cross section. The ion beam is parallel to the front and back wall and 7° tilted with respect to the surface normal. The quantity depicted is the logarithm of the integral of the dopand concentration over the coordinate perpendicular to the wall surface, divided by the implantation dose. The axis labeled "lateral" covers the lateral coordinate of all four side walls.