Two Dimensional Modeling of Implant Damage Effects on Impurity Diffusion

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Brief Abstract

A two dimensional process simulator using phenomenological diffusion models is described, and simulations of implant damage effects on impurity diffusion are compared to 2D profiles obtained by a chemical staining technique.

Extended Abstract

Submicron device technology is driving the development of a new generation of process simulation tools. The shallow junction depths and low thermal budgets of this technology imply that impurity diffusion is substantially controlled by the effects of implant damage and the annealing of this damage [1]. These effects, however, are nearly impossible to model in point-defect based simulators for a number of reasons. Such simulators require as initial conditions information about point defect generation and the evolution and distribution of damage layers. More importantly, the subsequent annealing of damage involves the dissolution of dislocation loops and point defect clusters. The parameters which determine the influence of implant damage and its annealing on the concentrations of point defects have not been determined theoretically or experimentally.

We present results of simulations of the impurity diffusion process using an extension of the phenomenological diffusion coefficients and the "deep decision tree" approach of PREDICT [2]. This allows us to model effects, such as implant damage, which are difficult to model with other two dimensional simulators. Phenomenological models are also used for the ion implantation and oxide growth steps.

Many of the diffusion models from PREDICT can be applied in two dimensions with minor modifications. The diffusion models which must be changed describe effects with spatial dependence: implantation damage, silicon amorphization, oxide growth and other surface effects. The extension of these models to 2D involves finding analytical expressions describing the regions involved and the fitting of those expressions to measured data. Those data are composed of both conventional 1D impurity profiles and 2D profiles. To obtain 2D profiles the lateral diffusion of the dopant is magnified mechanically by sawing and angle lapping, and the magnified junction contour is determined by chemical staining. The two-dimensional shape of the junction is reconstructed from the measured stained contour, and the diffusion profile is obtained by measuring the junction shape on a series of samples with varying substrate resistivities.

Since we choose to deal only with the diffusion of impurities, we are able to achieve substantial speed-ups compared to point-defect based simulators. We use an underlying finite-difference grid of rectangles, plus a set of triangulated rectangles near the $Si-SiO_2$ boundary. The oxide boundary is approximated by using an analytical "bird's beak" model [3]. The curve representing the oxide boundary is propagated in two steps. First it is propagated during a time dt using the analytical model. Then, in a

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tangential sweep, states along the curve are updated. Regridding occurs only in retriangulating around the oxide boundary, a set of $O(N)$ rectangles compared to the computational region of $O(N^2)$ rectangles.

The grid of rectangles plus triangles at the interface may be automatically refined in a self-similar fashion. In other words, the regions which are refined have an underlying finite-difference grid of rectangles plus triangulated rectangles at the interface. The solution is advanced in time by the Crank-Nicholson method (trapezoidal rule) which is unconditionally stable and second-order accurate in time and space. This *implicit* method requires the solution of a nonlinear system of equations at each timestep. The nonlinear system is linearized at each timestep by a Newton method.

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