A PRACTICAL MODEL OF INTERFACIAL IMPURITY FLUX FOR PROCESS SIMULATION

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With the developmets of submicron devices, 2D/3D process simulations have become necessary for process/device design. However, long CPU time has often limited the extensive use of the higher dimensional simulators. One of the easiest way to reduce the CPU time is to reduce number simulation of grids. However, the grid sizes around boundaries become larger, especially for curved boundaries, increasing numerical errors.

This paper first discusses the simulation errors due to the difference of the grid size. Then, a new model is proposed, which is effective to reduce errors and is simple enough to implement in the simulator. The effectiveness of the model is demonstrated by the applications to diffusion from doped material and also to predeposition.

By employing conventional model for interfacial impurity flux, significant errors arise due to the difference in the grid size. Fig.1 shows an exmaple in which the total number of impurities, S, introduced from doped oxide source into the silicon substrate are plotted vs.annealing time with the parameter of the grid size within SiO_2. S increases rapidly at the initial stage of annealing. However, after annealing time of about 0.01min, S saturates. The saturated value of S varies with the grid size, and is almost proportional to the grid size.

This can be explained by the difference of conventional interfacial flux(F_B) from the diffusive flux(F_D) in adjacent grids. When F_B is smaller than F_D, the simulation results do not depend heavily on the grid size. When F_B is larger than F_D, however, simulated interfacial flux depends heavily on the grid size, whichi is the case in fig.1.

In the practical case, F_B is usually larger than F_D as shown in fig.2. Here, D/h Y is plotted vs. Y at 1000°C. D/h Y smaller than unity indicates that F_D is less than F_B, causing grid-size-dependent simulations.

The outline of a new model is as follows. In addition to the known impurity concentrations at actual grids, impurity concentrations at imaginary points right at the boundary are guessed from the current concentrations at actual grids, and interfacial flux through these imaginary points is used for discretization instead of the flux through actual grids at the boundaries. It is noted that actual grids are somewhat away from the boundary because the box-type discretization implies that the grid is actually the center of mass of a cell. By modifying the known segregation and transport coefficients, discretization using only

the actual grids becomes possible, in which interfacial flux through the imaginary points are realized. Thus, the model can be easily implemented in any simulator.

The effectiveness of the model is demonstrated through the applications to impurity diffusion from doped materials and to impurity predeposition.

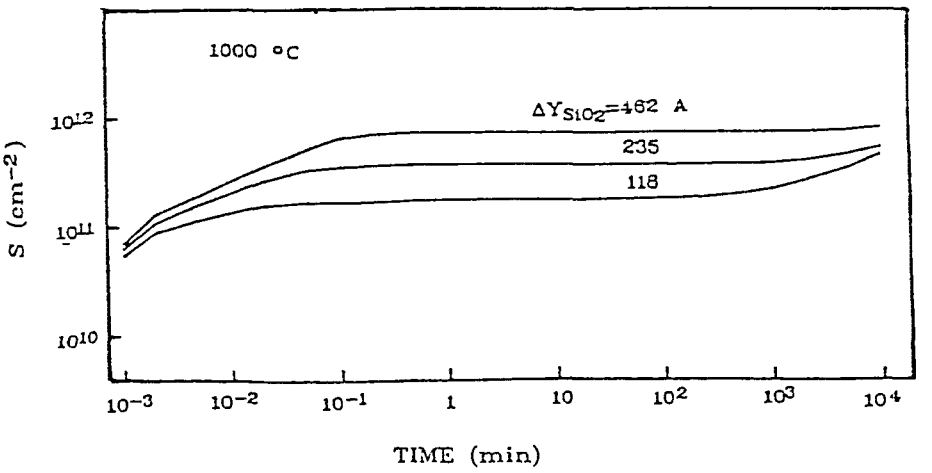

Fig.1:Simulation by SUPREM

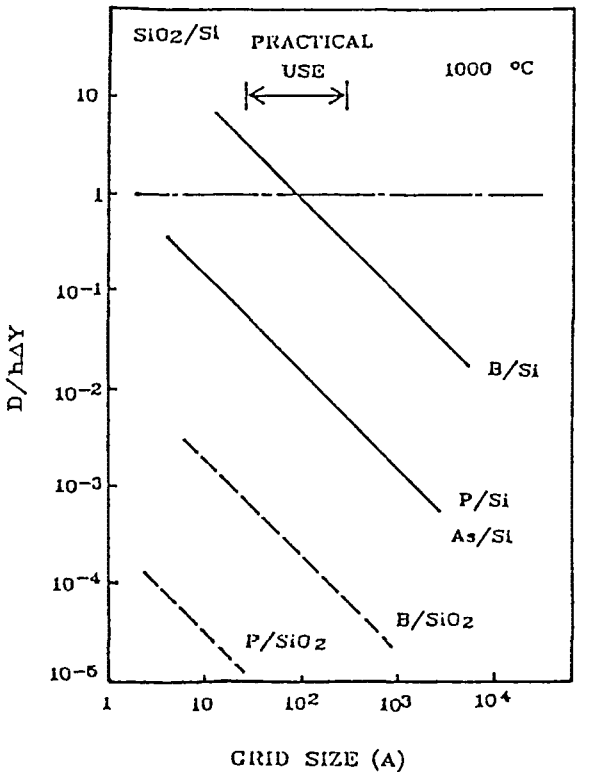

Fig.2:D/h Y vs. grid size