The Simulation of Lateral Oxidation Enhanced Diffusion using Coupled Point Defect and Impurity Diffusion Solutions

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The coupled diffusion of point defects and impurities is simulated efficiently in two dimensions using a coarse grid to represent the rapidly diffusing point defects and a much finer grid to resolve the details of the impurity profiles. The simulation results are fit to experimental lateral OED data to extract point defect diffusivity and interface recombination velocity.

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A program has been developed which efficiently solves the coupled diffusion of interstitials, vacancies, and multiple impurity species in two dimensions. Due to the vast differences in diffusivities of the point defects and impurities, two separate spatial grids are used. A coarse grid is sufficient to represent the rapidly diffusing point defects, whereas a much finer grid is necessary to resolve the details of the impurity profile. Independent time steps are automatically selected for each species, permitting this extremely stiff system of diffusion equations to be solved in acceptable CPU time on a minicomputer.

In this paper the simulation results are is used to study the coupled diffusion of interstitials, vacancies, and a single impurity species under local oxidation conditions. Comparison with lapping and staining measurements on structures with various widths of oxidizing and nitride masked regions allows values of point defect diffusivity, interface recombination velocity, and interstitial-vacancy reaction constant to be found. Significant conclusions from this study are:

1. Contrary to the assumptions of a number of previous authors, the time for point defects to reach their steady-state distribution can be many hours, requiring transient analysis for accurate diffusion simulation.

2. Under a silicon nitride masked region adjacent to an oxidizing region, the diffusivity enhancement can increase as a function of depth.

3. Due to different fractional interstitialcy components of diffusion, the oxidation conditions which minimize lateral impurity diffusion will be different for each of the commonly used dopants in silicon.

Figures 1 and 2 show the two-dimensional simulation of boron OED and antimony ORD after local oxidation.

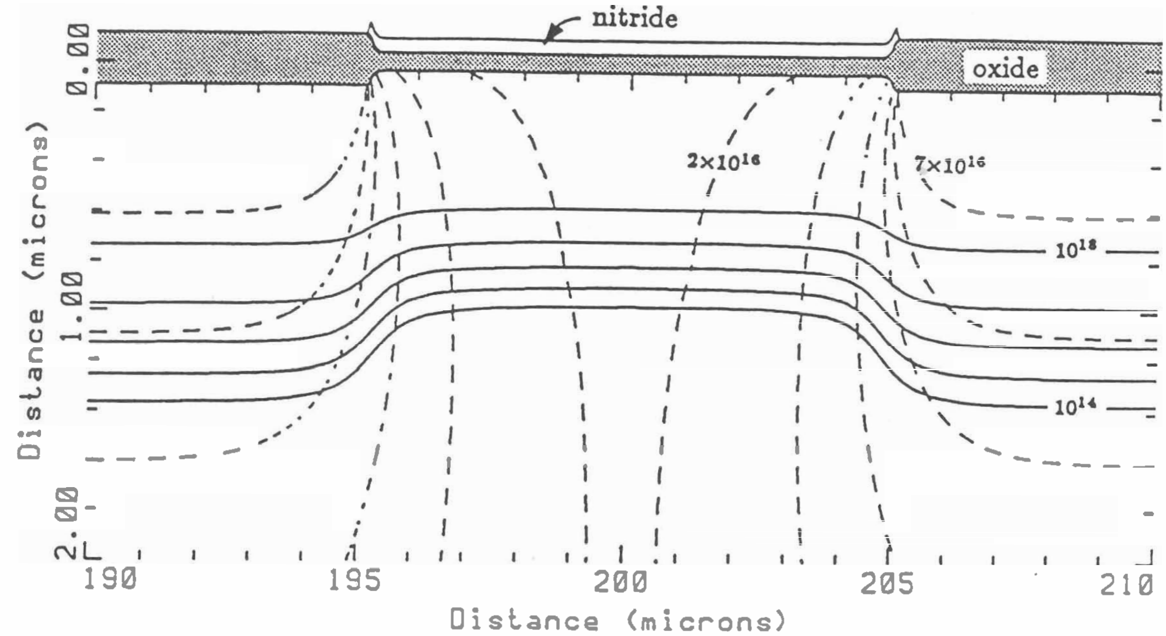

Figure 1: Interstitial (dashed) and boron (solid) concentration profiles after 24 hours of oxidation in a dry oxygen ambient at 900°C. At the center of the nitride masked region the interstitial concentration, and hence boron OED, is greatest at a depth of approximately 2 microns.

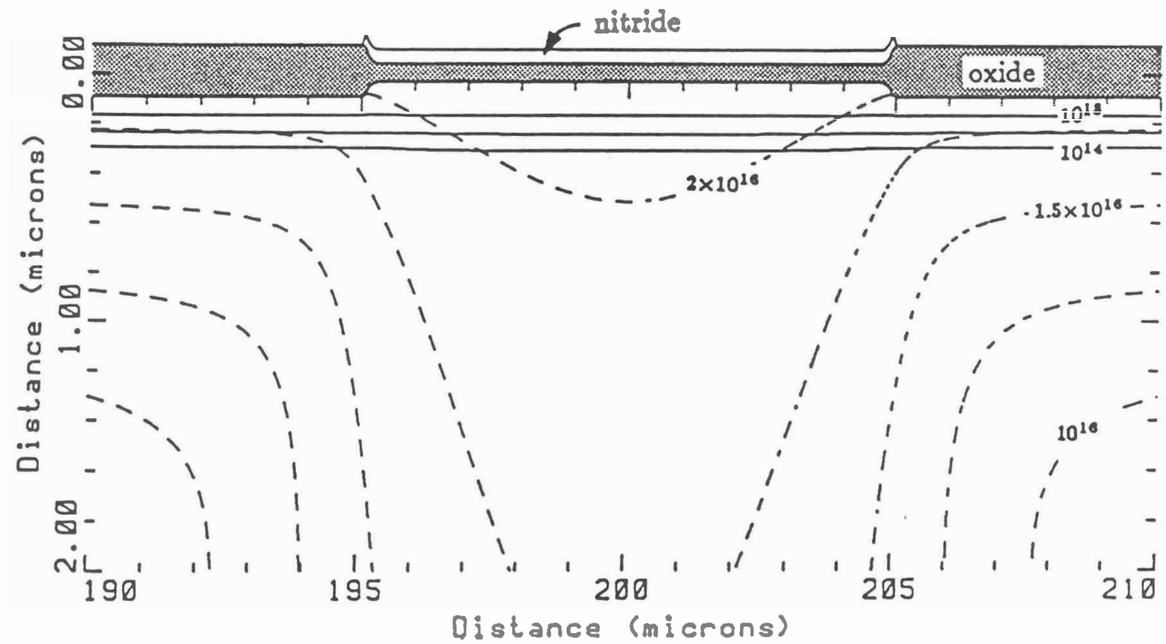

Figure 2: Vacancy (dashed) and antimony (solid) profiles for the same oxidation conditions as Figure 1. Due to vacancy injection at the oxidizing silicon interface the vacancy profile beneath the field oxide is maximum at the interface—the opposite from what would be expected if $C_I C_V = C_I^* C_V^*$ had been asssumed.