RTA-SIMULATIONS WITH THE 2-D PROCESS SIMULATOR PROMIS

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Anomalous diffusion during rapid thermal annealing has been successfully modeled in one space dimension using Monte Carlo simulations to determine the implantation damage and a kinetic five-species model to describe the diffusion process [1]. Straightforward extension to 2-D faces serious problems concerning demands on computation resources. To overcome these problems, we make two contributions in this paper: (1) We present an efficient algorithm for Monte Carlo simulations of point defect distributions arising from ion implantation in arbitrarily shaped 2-D structures. (2) We investigate the possibility of using an adaptive grid when profiles obtained by Monte Carlo simulations are used as initial conditions for diffusion simulations.

In the presence of an implantation mask, the damage distribution depends on the geometry and the composition of the mask. As RTA simulations depend critically on the initial conditions for the point defects, the simulation of point defect production during ion implantation in arbitrary structures is desirable. An efficient Monte Carlo simulator for the determination of dopant profiles in arbitrary structures has been presented previously [2,3]. The efficiency of this code is based on the multiple use of trajectories. A straightforward extension of this method to include point defect production would be to store whole recoil cascades and to use them several times. This would require significant amounts of data to be stored, especially if more than one target material is present. To avoid this problem, we store only one trajectory for each particle/material combination, and construct the recoil cascade from these trajectories (by "particle" we mean the ion or any target atom species). As a consequence, the cascade will reflect to some extent the peculiarities of the few stored trajectories. However, when many cascades, produced by different ions, are superposed, this effect will be smoothed out.

Using an adaptive grid is indispensable for 2-D RTA simulations in order to keep the number of grid points small. This cannot be accomplished by different, fixed grids for dopants and point defects, as the point defects evolve from a distribution which is confined to a small area, to a flat distribution. A typical initial point defect distribution obtained by Monte Carlo simulation is shown in Fig. 1. Two features can be seen: The profile is dropping to zero when the concentration falls below a certain value which corresponds to a single particle in a mesh element of the Monte Carlo simulation. Furthermore, there is considerable jitter at low concentrations. A grid criterion which resolves steep gradients (in the logarithmic scale) will move many lines to the vicinity of the jitter. As the jitter will be smoothed out in the early stage of the simulation, it is more important to conserve the local dose of the point defects and dopants than to resolve the gradients accurately. Therefore, a second grid criterion is used which conserves the dose [4]. These criteria, applied to the profile of Fig. 1, produce the grid shown in Fig. 2. We found that a good behaviour of the grid is fairly insensitive to the parameters of the criteria.

Simulations based on a pair-diffusion model [5], consisting of 5 equations for interstitials, vacancies, substitutional dopant, dopant-interstitial pairs, and dopant-vacancy pairs have been performed. As a test we used analytical functions for the initial profiles in one run and the same distributions with heavy jitter added in another run. We found no deviations of the results after physically meaningful times. In the second case some additional small time steps were necessary in the beginning of the simulation, which, however, did not contribute substantially to the execution time. We conclude that, although some smoothening of the Monte Carlo profiles might be desireable, remaining jitter is not detrimental to diffusion simulations using an adaptive grid.

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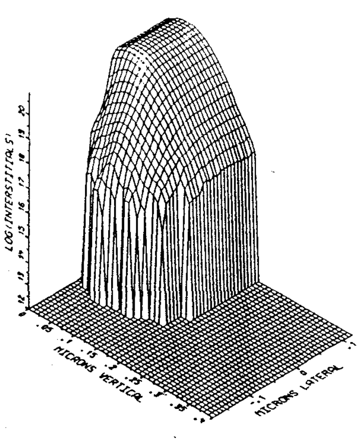

Figure 1

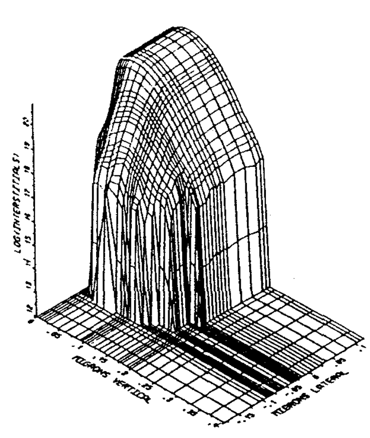

Figure 2