Multiscale Modeling of the Implantation and Annealing of Silicon Devices

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Process simulators for silicon devices are benefiting from recent work on several models that cover vastly different length and time scales. In this talk we will focus on molecular dynamics (MD) and Monte Carlo (MC) models. We will describe these models and the applications of the results to commonly used simulators such as SUPREME-IV and PROPHET. Improvements in these continuum simulators are presently being implemented by the introduction of mechanisms and energetics derived from the more fundamental approaches. We will discuss MD methods, which can provide some of the parameters needed for the rates of diffusion, recombination and other phenomena modeled by the simulators. The MC model is less detailed and can simulate entire implantation and diffusion cycles. It is also atomistic in scale, and gives results on the dopant density, clusters and other properties. In addition, the model includes stochastic effects of implantation and diffusion, which are of increasing importance as device components are scaled down in size.

Molecular dynamics (MD) simulations employ empirical interatomic potentials and classical dynamics to obtain the the trajectories of a small group of atoms. Of necessity, the methods are limited to small systems and short times; e.g., tens of thousands of atoms are simulated for several microseconds of elapsed time. This is sufficient time to simulate the initial damage to crystalline silicon resulting from ion implantation, and some diffusion events during annealing at high temperatures. An advantage of these simulations is their ability to reveal new mechanisms. The only input to the models is the empirical potential, which is often based on parameter-free electronic structure calculations. Thus, the dynamics are not constrained by the need to impose particular mechanisms, and often the simulations reveal unexpected phenomena. The formation energies of defects and binding energies between defects at low temperatures are also obtained using these methods. We discuss simulations by MD of the collisions of ions and clusters with silicon targets. We have investigated some of the effects of these collisions on the displacement and subsequent diffusion of dopant atoms, and on the extent and stability of amorphous silicon pockets created by the cascades. We also describe MD simulations of interstitial and vacancy diffusion, clustering, and recombination.

Monte Carlo models of the atomic displacements are a natural way to extend the

MD results to time and length scales appropriate for device processing. These models start with a configuration of defects and dopant atoms in silicon resulting from implantation. The implantation process is simulated either by MD, or by a binary collision approach. Our MC model is based on simulations of elementary diffusion hops which may lead to the recombination of point defects, clustering of point defects and dopant atoms to form clusters, re-evaporation from clusters, and other similar processes. It is parameterized using MD data and, if available, with data from first-principles electronic structure methods. Information from experiments on boron doped superlattices and other test structures is also used to verify and refine the model. The MC model contains a complete, up to date record on the condition of each defect and dopant atom present in the crystal during the annealing simulation. Using this information, the MC event selector is able is able to operate with high efficiency. As a result, it is possible to simulate the complete annealing of the defects caused by a 40keV silicon ion at a dose of 10^{14} in less than an hour on a fast workstation.

We will describe MC simulations of boron implantation and annealing under a wide range of conditions. The model predicts the the extent of transient diffusion, the distributions of the substitutional and clustered boron (active and inactive fractions), in good agreement with experiments [1]. The model can be used to explore processing conditions to optimize the boron distribution, and to maximize the substitutional component. In addition, we have studied the effect the mass of the implanted ion on the amount of transient diffusion. Large mass ions such as Pb cause extensive recoils in the silicon target, and the resulting diffusion of point defects produces more transient diffusion than would be expected from the "+1" model. Comparisons of the MC model with experiments show good agreement [2]. Other effects such as the dose dependence of transient diffusion are also explained by the model.

The power of workstations and improvements in code have reached the point where it may be useful to include MC simulators with the tools available for device design and process control. These simulators would provide more complete information on dopant and defect configurations, including correlations and other atomistic effects that may influence device operation.

References

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