Process Modeling for Submicron Silicon Technology
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1. Introduction
The progress of silicon process technology provides continual challenges for the development and refinement of process models. Existing processing steps require more accurate modeling, and models for new processing steps must be introduced if simulation tools are to keep pace with the demands of device design and process integration. The potential benefits are also increasing rapidly, since the development cost has been doubling for successive generations of technology.

Process modeling can be applied at several levels, from the highly detailed for analysis of a single processing step to the relatively undetailed for a rapid overview from the circuit layout level. We will concentrate on modeling at an intermediate level of detail appropriate for technology development, comparing our current level of understanding with the demands of submicron silicon technology to assess the status of process modeling today and the most pressing problems to be addressed.

2. Discussion
Processing steps can be divided into three broad categories: (1) lithography, (2) pattern transfer (deposition/etching), and (3) thermal processing and doping.[1] For the purposes of technology simulation, lithography can still be considered as an ideal process which produces resist patterns with almost vertical sidewalls. Exposure techniques and resist structures have improved along with the trend to shrinking linewidths to allow this view to remain sufficient. Simulation of deposition and etching is becoming more important, particularly where the topography is critical to later thermal or implantation steps, but modeling is still at the geometric level rather than from physical first principles. This is successful because the deposition/etching profile shapes are relatively well decoupled from other process steps so empirically adjusting coefficients to match a reference cross-section can give useful results. However, this is clearly an area where more physically-based models could have a significant impact.

Most of the effort in process modeling has been in the area of thermal processes and doping. This ranges from subjects that have been studied for many years, such as diffusion, oxidation and implantation, to those introduced into silicon technology more recently, such as silicidation and rapid thermal annealing. The drive towards reduced thermal budgets to achieve shallower junctions has required continued refinement of our physical understanding. In particular, understanding the role of point defects has been central to our progress, linking each of these processes together.

It is now generally agreed that both vacancies and interstitials play a significant role for dopant diffusion in silicon. These point defects form pairs with substitutional dopant, allowing it to diffuse through the silicon lattice. Fig. 1 shows an example calculation for diffusion of an implanted boron profile. The diffusion profile is the result of heavy doping modifying the fermi level leading to local enhancement of the point defect concentration, which in turn enhances the dopant diffusion. In addition, the various charge states of pairs formed allow some defect injection into the substrate where other dopant diffusion may be disturbed. The diffusion profile will be modified by any process which alters the point defect distribution: injection by oxidation, nitridation or silicidation; damage from implantation; differences in recombination kinetics in the bulk or at the surface. Explicit modeling of point defects and dopant-defect pairing helps give us insight into the processes that determine the final profile shapes. For submicron silicon technology, modeling of outdiffusion from silicide and polysilicon layers is also essential.

Implantation is still the method of choice for introducing dopant into silicon structures. The issues for modeling are the more accurate calculation of implanted ion profiles, considering channeling, shallow implantation angles at trench walls and surface films such as silicides, and the modeling of damage formation, both for its effect on channeling and for later diffusion calculations. Fig. 2 shows a two-dimensional calculation for the structure described by Izawa,[2] where the differences in lateral spread between the amorphizing silicon implant and the doping boron implanted led to unexpectedly large penetration of the boron under the gate. Our understanding of how
the damage from such an amorphizing implant should be incorporated into later diffusion calculations is far from complete. For channeling, although some models have been proposed, this is still an area where more investigation is needed both to improve the generality of the models and to make them suitable for repeated use in a technology simulator.

The use of recessed isolation, trench structures and lower temperatures pose the greatest challenges to oxidation simulation. Fig. 3 shows an example calculation for thin oxidation of a trench corner, and Fig. 4 the effect of the corner shape on the field distribution across the oxide. The local thickness of the oxide depends critically both on the initial curvature of the surface, and so on the quality of the etching model, and on the stress-dependence of the oxidation rate. Although there has been experimental work on oxidation of curved surfaces for relatively thick oxides, there is little data available for the thin oxide regime used in submicron technology.

REFERENCES

3. C. S. Rafferty, Private communication.