Process modeling for future technologies

by M. E. Law

Process modeling is an integral portion of technology computer-aided design (TCAD) and can be used to predict device structures and doping. Truly predictive process modeling has proven to be an elusive goal, because the controlling physics is complicated and difficult to investigate experimentally. The current state of process modeling is reviewed, and current and future challenges are discussed. Recent helpful trends are indicated, and problems that must be addressed are identified.

Introduction

As device lots become more and more expensive, the importance of technology computer-aided design (TCAD) is increasing. TCAD can be used to simulate device fabrication and performance and to avoid processing experimental lots. In the world of circuit design, CAD tools are frequently used to produce chips with working circuits on the first silicon fabrication lot. In theory, TCAD could be used to produce a new process that also works on the first try. In practice, however, TCAD falls short of this goal.

TCAD comprises many elements, including equipment simulation, pattern transfer simulation, and compact modeling. However, the two main components have been process simulation and device simulation. Process simulation predicts the structural and doping profiles of the device on the basis of the key processing parameters, e.g., implant dose, energy, and anneal time and temperature. This structural information can then be used as input for device simulation for prediction of the electrical device behavior.

Process simulation has typically been the weaker element of TCAD. Device simulation has become quite sophisticated and surprisingly accurate for today's superscaled devices. However, although the sophistication of process simulation is increasing, its accuracy remains a problem. There is generally a time lag between the introduction of a particular process and its accurate modeling—the problem of "yesterday's technology modeled tomorrow." However, for many problems, absolute accuracy is not required. Relative trends provide excellent information about the process in question.

Technology scaling has traditionally provided bigger challenges to process simulation than to device simulation. Originally, junctions were diffused in from a solid source and then diffused to a desired depth. This process could be computed and predicted from analytical functions. In time, however, solid-source diffusions were replaced with implanted junctions. These implanted junctions offered an entirely new modeling field (see for example the review by Gibbons [1]). Since local oxidations were used for isolation, it was discovered that surface reactions changed the diffusion of the underlying dopant layers [2]. With reduction of temperature and time cycles, it was discovered that diffusion was not constant in time, and was affected by the damage from the implant process itself. Modern anneals are done without a furnace; they

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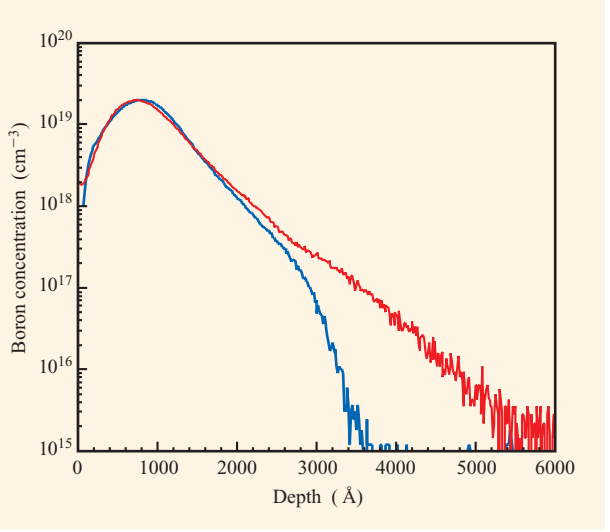

Figure 1

Boron as implanted (blue) and diffused (red). There is a clustered, immobile region near the peak (containing {311} defects, dislocation loops, boron–interstitial pairs and clusters, and trapped and free interstitials) where the damage is highest. The tail is spread out by transient-enhanced diffusion. The evolution of the profile is dominated by the extended defects, boron–interstitial complexes, and interstitials.

are performed in a rapid thermal annealer (RTA). RTA processes today rarely use a period of fixed temperature—they just spike up to a temperature and then cool rapidly. Each innovation in technology has required process modeling tools to work with new dominant physics and new processing technologies. To accurately predict results requires extensive characterization of the underlying physical phenomena.

This paper focuses on the prediction of junction formation technologies and the prediction of doping profiles. This tends to be the largest problem area for predictive process simulation, and certainly exemplifies the problems that can arise. The paper reviews the current state of the art in dopant modeling and discusses some of the reasons for the time lag between the introduction of technology and accurate modeling. It then explores future trends and examines the techniques that might allow this gap to be closed.

Primer on junction formation modeling

The modeling of dopant profiles in the current process consists of modeling the ion implant process and then modeling the anneal cycles. Implantation has been used in device fabrication for more than 20 years to introduce dopants into the substrate silicon. Annealing has been used to repair the damage from the implant. Through the years, implant energy and temperature cycles have been significantly reduced. Typical annealing times today are several seconds.

There are two major challenges in modeling the junction formation process. First, we need to predict the active, substitutional concentration of the dopant, since only the active concentration contributes to the electrical properties. The other challenge is accurate prediction of the diffusion profile, which in most cases determines the junction depth. The junction depth and steepness also determine the electrical properties of the device.

At first glance, this does not appear to be a complicated system to solve. Ionic stopping in solids is fairly well understood, and solid-state diffusion is a well-characterized problem. However, the common dopants in silicon are tightly bound when substitutional, and do not diffuse by themselves. They require an interaction with a lattice point defect, either a vacancy or an interstitial. The dopants pair with the defects to form a mobile species. Consequently, the apparent diffusivity of the dopant is proportional to the local point-defect concentration in silicon. (For an excellent review, see Fahey et al. [3].) The implantation creates a large amount of crystal damage, which appears initially in the form of vacancies and interstitials. As the damage is annealed, the diffusivity of the dopant changes dramatically. This process is called transient enhanced diffusion (TED). The complexity increases as the dopants and point defects form clusters that deactivate the dopant. Predicting the interaction of the damage with the dopants is extremely challenging, particularly since there are no effective ways to directly measure the point-defect properties in the silicon. The junction depth and activation of the dopant layer both depend on the point defects, which are produced in large concentrations from the implant process itself. **Figure 1** shows a boron profile in silicon after annealing. Most of the dopant in the peak region has clustered. The tail is spread out by transient enhanced diffusion, forming a deeper junction.

Modeling the implant process requires an understanding of how ions come to rest in the silicon substrate. The ions lose energy to the crystal in two ways. The ions can experience nuclear collisions with the lattice ions. Typically, this displaces the lattice ion, creating a vacancy and an interstitial. The lattice atom recoils with an energy that is frequently sufficient to create other recoils. The implanted ion can also lose energy to the electronic cloud present in the crystal. The positive charge of the ion tends to accelerate the electrons in the vicinity, which creates a drag force on the ion. Electronic stopping does not create crystal damage. Since the collisions have a random nature, the profile ends up with a statistical distribution.

The oldest and most popular technique for modeling implant processes is based on using the moments of the

distribution from a table. The project range and standard deviation of the profile are used to predict a Gaussian distribution of the ions. For many cases, the measured profile does not look Gaussian, and various other distribution functions are used to fit the profile [4, 5]. Since the crystal has a regular repeating lattice, collisions are not really random. Some ions find the crystal channels and experience few collisions. This channeling profile is often added to the random profile, so that the total profile is a summation of the random component and the channeled component [5, 6].

This technique produces very accurate one-dimensional profiles, since they are fitted to the measured profile. However, there are several very large drawbacks to this approach. First, it is an approach that fits function to data. Attempts to model a profile outside the measured results are unlikely to be very accurate. This technique is not predictive—it requires the experiment to be performed before modeling is possible. Second, obtaining an accurate lateral profile under a mask edge is difficult. The lateral standard deviation of the profile is not necessarily the same as the vertical. The lateral channeling is very difficult to predict. Finally, this technique provides no information about the total damage and whether the crystal has been rendered amorphous. As pointed out earlier, accurate prediction of the damage is very important in predicting the annealing. Despite these drawbacks, moment-based modeling is still the most widely used technique for implants, and this limits the predictability of process simulation as a whole.

Solutions of the Boltzmann transport equation that can be applied to ion implantation address many of the drawbacks of moment-based techniques. Direct solutions are possible [7–9], but Monte Carlo calculations are generally used to solve the equations [10–12]. Monte Carlo simulation follows an individual ion on a trajectory through the silicon crystal. Random numbers are used to generate collision events. By tracking a statistically significant number of ions, this technique can be used to predict the ion distribution. If the interactions among the ions, crystal electrons, and lattice atoms are well characterized, a Monte Carlo code can accurately predict the profile that will result from any combination of implant parameters, dose, energy, implant angle, etc. Since it is not necessary to do the experiment first, it can be a predictive technique.

Monte Carlo simulation can also track the total damage [13–16]. By tracking the ion collisions, it can determine the primary damage. By following the recoiled lattice atoms, it can also tabulate secondary collisions. In principle, it is possible to predict the total damage generated and its position in the structure. It is also possible to compute the distance the ion travels perpendicular to the surface normal in order to understand the lateral distribution of ions.

Modeling of annealing requires a knowledge of point-defect behavior in silicon. The point defects, interstitials, and vacancies recombine, eliminating damage. Both point-defect species can cluster, and frequently interstitial-rich extended defects are observed [17–20]. As the defects recombine and cluster, they can also interact with dopants. Dopants can form mobile defect–dopant pairs or immobile higher-order clusters [21–26]. All of these interactions can create a vastly complex system, with a large number of reaction rates, binding energies, and diffusivities that have to be parameterized. The resulting set of nonlinear, stiff partial differential equations can be solved with a variety of numerical techniques.

Characterization of the parameters for the system of equations is a primary challenge. Point defects cannot be measured directly, so their behavior must be inferred from other experimental results. This means that experiments must be carefully designed, and that different parameters are obtained depending on the interpretation. This leads to controversies that are difficult to resolve. For example, a long debate was held on whether interstitials contributed to diffusion of the common dopants in silicon. Interstitial diffusivities have been reported with values in a range of six orders of magnitude [27–31]. An approach to obtaining the parameters is to use first-principles physics calculations [32–34]. These calculations can provide insight into the binding energies of various complexes and the migration energies of the mobile species.

Recent process simulation tools offer what has become known as the "dial-an-operator" approach [35, 36]. These codes allow users to enter partial differential equations on the command line so that sophisticated and complex models can be developed simply and easily. This development has sped the implementation and development of new models by allowing workers with no significant experience in software development and finite element techniques to implement modeling ideas.

Current challenges

The primary challenge of process modeling is to predict how the damage interacts with the dopants. Excellent work has been done on predicting the location of dopant ions from the implant, but less progress has been made on the evolution of damage during the implant and subsequent anneal.

Monte Carlo simulations can predict the amorphous layer [15]. The layer thickness can be measured with a variety of techniques, so it is easy to verify. However, there is incomplete understanding of the phase transformation from crystalline to amorphous material. Above a threshold damage concentration, it is thought that the crystal relaxes to a lower-energy state by

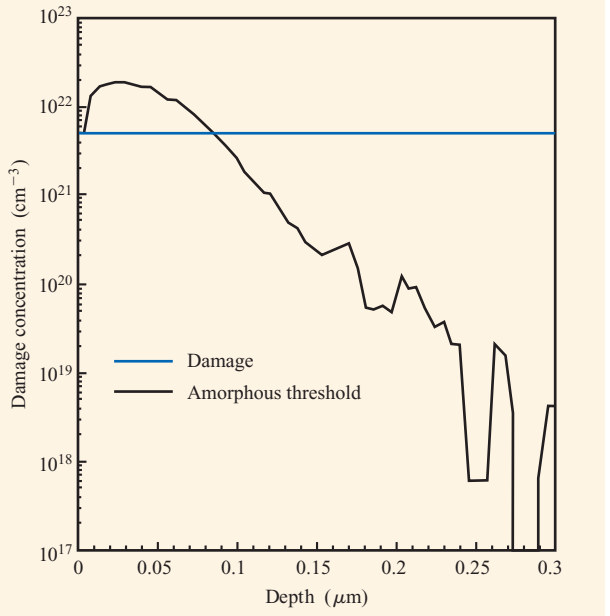

Figure 2

Damage profile from a 10^{15}-cm^{-2} 40-keV silicon implant. The threshold of the amorphous phase is shown in blue. This simulation predicts an amorphous depth of 83 nm.

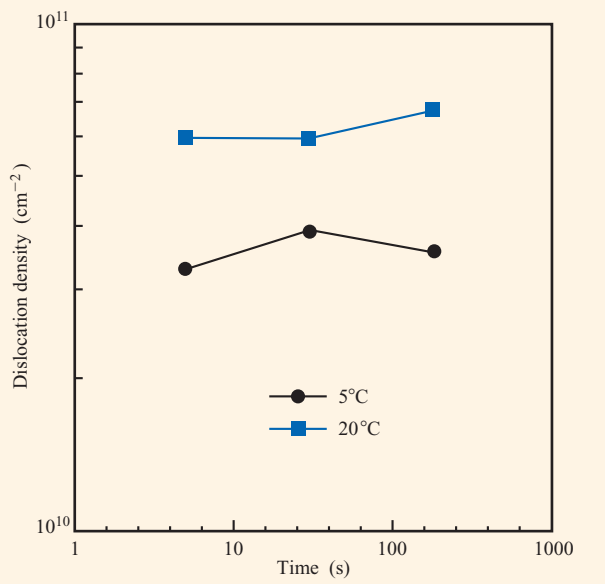

Figure 3

Defect density of dislocations as a function of implant temperature (5°C and 20°C) and anneal time at 800°C. The interstitials contained in the dislocations are about the same for the two implant conditions.

becoming amorphous. The threshold damage concentration is generally accepted to be at 10% of the lattice concentration, 5.0×10^{21} cm^{-3}. Because the damage profile falls off rapidly (**Figure 2**), a small error in the threshold damage density makes only a small change in the amorphous depth. In this example, a change in the threshold damage density by 10% creates only about a 5-nm change in the amorphous depth. Consequently, it should be easy to predict.

Unfortunately, this process is complicated because of dynamic annealing during the implantation step. Small variations in the implant conditions can alter the final damage profile significantly. For example, variations in the implant wafer temperature and dose rate can create changes in the depth of the amorphous layer and evolution of the end-of-range damage [37–42]. This can have significant effects on the remaining damage in the region beyond the amorphous crystal interface. Small changes in the amorphous depth, since the damage profile is changing rapidly, can create large differences in the total damage remaining beyond the interface. Beyond the amorphous depth, a large amount of damage exists. Molecular dynamics simulations of a single ion implanted into silicon indicate that the damage largely anneals and forms defect clusters [43]. Further complicating this behavior is the fact that the vacancy defect is mobile at room temperature, and free vacancies are not found in the crystal.

During the subsequent anneal, the damage evolves into extended defects. The evolution process is influenced by the implant temperature and dose rate. **Figure 3** shows the effect of implant temperature on the number of defects formed [44]. This data clearly shows that the nucleation of defects depends on the implant temperature, since there is a difference of about a factor of 2 in the density. The same numbers of interstitials are contained in the loops for both implant temperatures. It is likely that the defect nucleation occurs during the implant process itself. To date, no model for this behavior has been proposed, despite the fact that the extended defects are a source of interstitials for TED.

Another area of concern is the controlling factors for solubility. Since the technological push is to increase the active concentration to lower sheet resistance, understanding how the dopant is activated is critical. Traditionally, the principle of thermodynamic equilibrium solubility has been applied. For short-time-spike anneals, this is probably not useful. We need to develop understanding of the initial activation level of the dopant after the implant, and then to understand how further activation or deactivation occurs.

The process of doping with boron is fairly well understood. It is widely accepted that boron clusters into immobile boron interstitial complexes [23, 26]. At short times, boron forms interstitial-rich clusters that alter the damage formation. At longer times, these clusters become boron-rich and are difficult to break up. Doping with arsenic is less well understood. At intermediate dose levels, the arsenic forms clusters centered on vacancies [21, 45]. At higher doses, arsenic forms larger precipitates, and the character of the defects seems to change [22, 46]. The kinetic rates for both processes must be fully understood in order to maximize the dopant activation. The characterization of these behaviors is a critical near-term challenge for junction profiling.

Scaling challenges to modeling

Future device scaling presents several new process modeling challenges. First, the silicon oxide interface is well understood and characterized. We have good models for dopant segregation and trapping at the silicon/oxide interface [47], and understanding of how point defects behave. Device scaling will require the gate oxide to be replaced with a material with a higher dielectric constant.

Since the silicon/oxide interface is a strong sink for point defects, it has an important influence on the evolution of the damage profiles. When the oxide is replaced with a new material, the new medium must be rapidly characterized for its effect on doping profiles. This is one of the reasons why it is difficult for process modeling activity to become predictive. Currently it is not clear what material will replace oxide as the gate dielectric. Once the material is identified, experimental work to characterize the interface with respect to its effect on dopants and defects will begin.

A number of techniques can be used to characterize the surface. Dislocation loops dissolve by releasing interstitials, and are controlled by diffusion to the oxide interface [48]. Repeating the experiment with the new gate material will determine whether the new material is as strong a sink as oxide. Another clever experiment has been performed with a series of stripes of varying dimension [49]. Open areas were damaged, and the extent of lateral diffusion under the stripes was determined. The surface recombination of defects controls the extent of the lateral diffusion.

Another major challenge is to lower the sheet resistance of the source and drain junction while simultaneously lowering the junction depth. This is required in order to control two-dimensional effects in the transistors and to make sure that the dominant resistance in the device is the channel resistance. This is a difficult challenge to technology, and it may bring about the end of implant and annealed junction technologies. The *International Technology Roadmap for Semiconductors* (ITRS) suggests that future devices will have sources/drains that are grown or are laser-annealed. These processes can create higher activation through the phase transformation involved. For example, laser melting upon cooling can leave behind active concentrations at well above solid solubility. It is also possible to use low-temperature anneals to regrow the crystalline layer from amorphous material. During the regrowth, the dopant is incorporated in much larger numbers than equilibrium at the anneal temperature would dictate.

Although the kinetics of phase transformations are reasonably well understood, there are no good models that can predict the amount of dopant incorporated on lattice sites during the process. Because of this, TCAD is unable to answer fundamental questions about the level of activation resulting from the phase transformation. As these technologies are adopted, extensive amounts of work will be required in order to characterize the dopant behaviors. Unfortunately, much of this work cannot begin until the correct candidate technology is identified, which means that models will probably not be available until after the process is in production. It also means that much of the effort that has gone into understanding implant and anneal processes will not be as important for future technologies.

These are just two examples of challenges that will arise as technology advances. Keeping pace with Moore's law requires considerable innovation in process technology. In the next ten years, considerable changes in materials and process are going to be adopted by the industry. It will be extremely difficult for process modeling to keep pace with changes in technology. Each new material and process will have to be characterized in order to be modeled successfully, and for the most part, this characterization will be too detailed and extensive to fit the new technology into the process flow.

Future perspective of process modeling

There are several encouraging trends for process modeling. First, as mentioned earlier, there is a move to tools with scripting interfaces to provide partial differential equation support. This can increase the number of workers developing and characterizing models. However, making the models work together remains a daunting task, since there is still no agreement on the basic interstitial and vacancy parameters. A model may work with one set of parameters but not with a different set without retuning. A database of experimental results and techniques must be developed to allow models to be calibrated, but this will probably not happen outside individual companies.

Another trend is the increased use of atomistic tools in developing and characterizing models. *Ab initio* results can provide insight into formation and migration energies, and

molecular dynamics can further illuminate the dominant species and clusters. These first-principles calculations allow model development with significantly fewer parameters. The accuracy of these calculations must be carefully assessed, since it is easier to obtain energies than it is to obtain prefactors. It is hoped that the use of these tools will allow faster and more physical model development. For example, a recent model for nitrogen diffusion and segregation to the oxide/silicon interface was developed by using *ab initio* calculations [50].

There are also some problems to be addressed. Traditionally, process simulators have been developed in the university community, commercialized by vendors, and sold to semiconductor companies. This has been a slow pipeline, and there has been a considerable time lag between the development of model ideas in universities and their transfer to commercial codes. The use of scripted models could accelerate the pipeline, although vendors will still need time to be able to support models.

There is less funding for university research in this area, since the federal government has decreased its funding for silicon semiconductor research and industry has not made up the difference. Funding from the Semiconductor Research Corporation (SRC) has decreased in inflation-adjusted dollars, and the SRC is moving money from technology and devices to circuits and systems. Although the Microelectronics Advanced Research Corporation (MARCO) has increased funding for silicon and circuit research, none of the money has been oriented toward modeling activities.

Conclusions

Process simulation plays an important role in technology development at many companies, even if it is not always predictive. Locally tuned models can be important for diagnostics and for pointing the correct path for technology development. The fast pace of technology development makes it difficult for process simulation to be predictive, but there are signs that the model development process can be made faster and more accurate.

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