Technology computer aided design characterization needs and requirements

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Technology computer aided design (TCAD) promises predictive calculations of both structural and electrical parameters of advanced semiconductor devices. How realistic is this promise for shallow junction technology? What are the models used for predicting shallow junctions? What kind of verification and experimental support is required? Does TCAD place additional requirements on the characterization community? © *1996 American Vacuum Society.*

I. INTRODUCTION

Technology computer aided design (TCAD) is the software tool set that allows integrated circuit technologists to develop new processes and devices without having to build costly test lots. It is hoped that TCAD can provide the process engineer with the same benefits that electronic circuit CAD (ECAD) has provided to circuit designers. Circuit designers can design, lay out, and test new circuits without fabrication and largely be assured that the circuit will work when manufactured. This type of reliability is not yet available for TCAD users, and characterization of the models represents one of the key challenges.[1] There are three major components to TCAD: (1) small circuit simulation; (2) device simulation; and (3) process simulation. Process simulation is software that models the manufacturing process and predicts structural data. In this article, we will examine the needs of process simulation as they relate to shallow junction technologies.

In most of these TCAD areas, there is a range of models that provide complexity, accuracy, and computation time tradeoffs. For example, in device simulation there are many levels of simulation complexity available. There are circuit level empirical models, drift-diffusion simulators, energy balance codes, full hydrodynamic solvers, and finally Monte Carlo techniques. (For a review, see Ref. 2.) This range of models allows quick, empirically characterized models to be used in initial designs, and more complex, computationally intense models to be used for more challenging problems and physical insight. The range of models also allows self-checking, i.e., a complex model can be used to examine the worth and usefulness of an empirical model. The reverse can also be done, as a complex, first principle model needs to reproduce the empirical model where the empirical model is accurate and well characterized. Unfortunately, this is not the case in the area of shallow junction modeling and the major culprit is a lack of accurate, inexpensive characterization technology.

II. MULTIPLE DIMENSIONAL MEASUREMENTS

For device simulation, the simplest models were always the first to be extended to account for additional dimensionality. The first two-dimensional device simulators solved simple equations and evolved to include greater complexity. It can provide rough first estimates of the behavior of the new structure. As insight is gained with empirical models, more physics was added. Concurrent with this development, device simulation began to move to three dimensions.

For multidimensional device simulation to be accurate, there needs to be multidimensional doping profiles. Simple empirical models (Gaussians, Chebyshev polynomials, etc.) could be tuned with measured data to provide crude first-order estimates of the profiles for use in device simulation. This worked reasonably well in one dimension, as profile data could be easily obtained and fits could be obtained. It was not without flaws, however, and these will be addressed in later sections. Multiple dimensions are, however, another story entirely.

There are no cheap, widely used methods for two-dimensional profile characterization. The author believes this simple fact has kept TCAD from fulfilling its promise and becoming indispensable in process development. Without two-dimensional measurements, there can be no reliable two-dimensional empirical models. Consequently, the modeling effort has focused (nearly exclusively) on very physical models that are tuned to one-dimensional measurements. The *hope* is that if the physics can be verified in one dimension, it will scale appropriately to higher dimensions.

Several structures have been used in the past to examine two-dimensional diffusion behavior. One of the most popular, used first by Lin,[3] uses a variety of masking stripes. Figure 1 shows the structure. Conditions in the open area leak into the lateral areas, and the junction depth at the center of each mask can be measured with staining. This provides information on the lateral decay length of the phenomena in the open areas. Experiments of this type have been key in determining parameters for diffusion models. However, they provide limited information on the profile shape and give only crude indications of the diffusion behavior.

III. IMPLANT MODELS AND CHARACTERIZATION NEEDS

During ion implantation, the ions enter the crystal and experience two types of energy loss. The first is a loss to the electron cloud, which is somewhat uniform in space. The

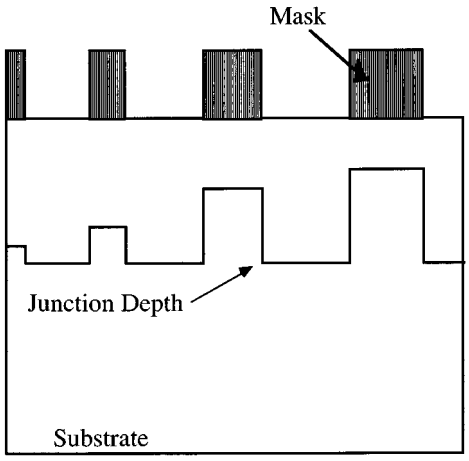

FIG. 1. A diagram of a stripe experiment. If conditions are altered in the open areas, it can create changes laterally under the mask regions.

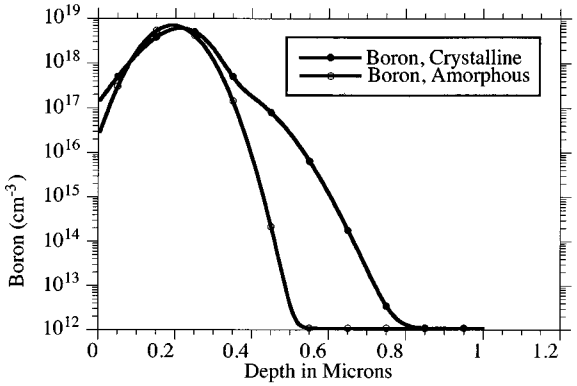

FIG. 2. Boron $10^{14}/cm^2$, 60 keV implants modeled empirically into amorphous (no channeling) and crystalline material (channeling).

nonuniformity comes from the unequal electron density as a function of position in the crystal. The second loss source comes from nuclear collisions between the crystal atoms and the incoming ion. These are highly random and depend on the ion energy and momentum vector in the crystal. Some implanted ions enter the channels of the crystal, and the nuclear loss mechanism becomes nonexistent. These ions ''channel'' much deeper into the crystal than those randomly oriented. As the number of collisions increase, crystal damage accumulates and the probability of finding a clear channel decreases. The number of ions that channel is a strong function of the accumulated damage in the crystal.

The empirical approach for implantation makes use of the statistical nature of the energy loss process. Statistical functions (Gaussians, Pearsons) are used to represent the distribution of ion stopping places. Measurement of implanted profiles allows characterization of the statistical function, and a great volume of this data has been accumulated and stored in look-up tables. Typically, these tables are indexed by energy and the profiles are then scaled by the dose.

Superficially, this seems to be an outstanding approach. However, there are several limitations. First, channeling is very difficult to include. Since channeling depends on dose, the statistical functions cannot be simply scaled by the dose—the parameters in the function must have a dose dependency. The channeling can be a significant component of the profile. Figure 2 compares a boron profile for an amorphous silicon layer (no channeling) with its single-crystal equivalent. Figure 2 shows a large difference between the profiles, which indicates that the ignoring channeling is a substantial error. In addition, the channeling depends on screen oxide thickness, implant angle, and sample rotation. Excellent fits have been obtained using dual-Pearson functions.[4] However, the data required to parametrize these models becomes quite large, and requires many man years of effort to obtain. The characterization challenge is enormous, particularly as technology trends are factored in.

Second, the lack of any inexpensive two-dimensional characterization limits this approach. The lateral implant straggle can be characterized with more sophisticated simulations,[5] but then the data base suffers from any inaccuracy there may be in these simulations. As discussed earlier, the lack of measurement technology can severely cripple the accuracy of the empirical model.

Interestingly, recent numerical experiments have shown that this approach begins to lose even the computation advantage in multiple dimensions. Since the statistical function used in the point response of the implant, the point response must be integrated across the surface of the simulation space. In two dimensions, there is a suitable analytic solution for sections perpendicular to the implant beam. Unfortunately, no such simplification exists in three dimensions, and the profiles need to numerically integrated across the surface. This process can consume significant CPU time that is on the order of the solution of diffusion equations.

The second major approach for implant modeling is to simulate each ion entering the crystal, and to use random numbers to determine its interaction with substrate atoms, known as Monte Carlo. Each ion is followed individually, and a large number of ions is used to provide a statistically significant sample. Random numbers provide the chance of collision and the impact parameters for the collision. Monte Carlo is computationally complex, and is not in widespread use for technology development.

The parameters required for Monte Carlo simulation are atomic level and difficult to measure. For example, one key parameter is the collision cross section of the crystal atoms and the energy loss function for collisions within this radius. Direct measurements of these parameters are not available. It is hoped that they can be obtained from first principles, but this has not always produced parameters that agree with experimentally observed profiles. Usually, parameter tuning is performed to obtain better agreement with observed one-dimensional measurements.

A great challenge for implant characterization is measurement of the damage profile produced by the implant. This is a key variable for modeling the channeling results, and has significant impact on the diffusion models. At present, there

is no method of characterizing damage. It is possible to measure the onset of amorphization as a function of dose, but this provides only crude information on the damage production. Channeling reduction can only be inferred from measured profiles' dependence on dose, and the Monte Carlo method loses some of its predictive capability. This will turn out to be a critical part of the anneal model for shallow junctions.

IV. DIFFUSION MODELS AND CHARACTERIZATION NEEDS

As with implantation, there have been two primary mechanisms for simulating diffusion behavior. Both rely on solving a continuity equation for the dopant numerically, but have different approaches for modeling the diffusivity. The first is a phenomenological approach, for example, the decision tree simulator PREDICT.[6] This program uses a decision tree based on implant and annealing conditions to pick the diffusivity to use for each dopant. The diffusivity is allowed to be time variant. Simple empirical expressions for the diffusivity were derived based on empirical evidence and physical insight. In theory, this approach should be extremely useful. It is the equivalent of drift-diffusion device modeling, where the mobility becomes an empirical fitting expression.

However, the approach is limited by both the available data and its accuracy. Since the technique is based on empirical extraction of the diffusivity, the models have limited predictive validity outside the region of validation. Consequently, experimental verification and calibration must be performed before the models can be used. This is true of all empirical approaches, and is not meant as a criticism of the approach. It does, however, require a substantial commitment to the characterization of the junctions in the design space.

Accuracy is a critical issue, because the extraction of diffusivity from a measured profile can produce large error bars even for excellent measurements. This can produce large difficulties when interpreting results and extrapolation of results to new times and temperatures. Consider a Gaussian profile,

$$C(x)=\frac{Q}{\sqrt{\pi(Dt+\sigma)}}\exp\left(\frac{-x^2}{4(Dt+\sigma)}\right),$$

where Q is the initial dose, σ is the initial squared standard deviation of the Gaussian, x is the depth, and Dt is the diffusivity time product. As an example, consider boron with an initial dose of $10^{14}/\mathrm{cm}^2$ and an initial sigma of 1.32×10^{-13} cm^2, that result in an initial junction depth of 0.2 μm. If we anneal this profile for 60 min at 900 °C, the junction depth will increase to 0.234 μm, assuming an inert diffusion behavior. This translates to a diffusivity time product of 6.71×10^{-14} cm^2. If the measurement is accurate to 50 Å, the error in the diffusivity is $\pm12\%$. This error is increased when you consider that the profiles produced are not noise free, and the best fit Gaussian profile can be debated.

The other main modeling approach is based on the underlying physical processes. Dopants diffuse through interaction with point defects, and the point defect equations can also be solved. The defect concentrations are then used to compute the local dopant diffusivity. As the defect concentrations change and evolve, so does the dopant diffusivity. This allows a first-principles type of approach to diffusion modeling. The model equations are complex, and typically look something like this:[7–9]

$$J_A\equiv\sum D_{AX}C_A^+\frac{C_X}{C_X^*}\nabla\log\left(C_A^+\frac{C_X}{C_X^*}\frac{n}{n_i}\right),$$

$$J_X\equiv D_XC_X^*\nabla\left(\frac{C_X}{C_X^*}\right),$$

where J is the flux, C is the concentration, D is the diffusivity, the subscript A is the dopant, the subscript X is the defect; interstitial or vacancy, the superscript + represents the substitutional quantity, the superscript * is the equilibrium concentration, and n/n_i is the electron concentration divided by the carrier concentration. The term D_{AX} in the first equation is the weighted diffusivity due to the dopant-defect pair. The summation is over both defect types and all defect charge states. Using this system requires three partial-differential equations to be solved to account for the motion of one dopant species, and therefore can be computationally complex. In theory, these systems of equations can predict dopant behavior under a wide variety of conditions.

This system is not without drawbacks and there are several main ones. First, there is an explosion of parameters required, many of which cannot be independently determined. Second, point defects cannot currently be measured directly. Third, there is a cyclical process to parametrizing and characterizing the models. All of these represent characterization challenges.

Introducing two additional partial-differential equations means that there is a vast increase in the number of parameters. We now require knowledge of the defect diffusivities, defect equilibrium concentrations, recombination rates, boundary conditions, and charge states. This wide variety of parameters represents an increase in the characterization space. It is also made worse, since a physical model is only as accurate as the physics included. Leaving out any major physical effect can create significant errors. In diffusion modeling, there also seems to be sort of an inverse Occam's razor operating in diffusion modeling—Occam's hammer. Occam's hammer states that if a complicating effect can be thought of, it should be included because it will eventually be important as technology shrinks. As the modeling of diffusion has advanced, more and more effects and interactions have needed to be added to the models in order to continue to include the full physics of the model. This increases the burden on parametrization efforts.

The preceding problems would not represent a major roadblock, except that the defects cannot be measured directly! This means clever experiments must be designed to calibrate the defect models. Interpretation is difficult at best, and has led to lengthy debates about various basic concepts. For example, years were spent debating the question, ''Do interstitials play a measurable role in dopant diffusion in sili-

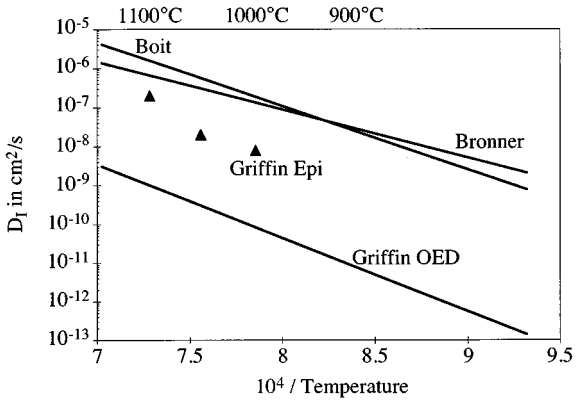

FIG. 3. Values of the interstitial diffusivity extracted from different experimental conditions.

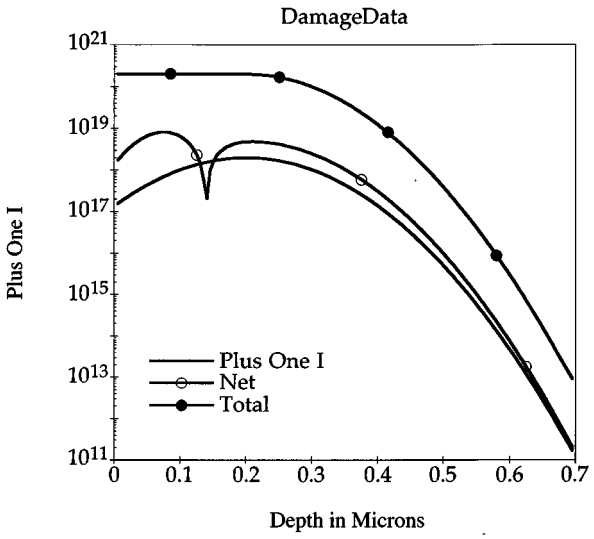

FIG. 4. Damage concentration assumption for several different models.

con?'' Fundamental properties of the defects become subject to great controversy and do not find widespread agreement within the modeling community. For example, Fig. 3 shows the interstitial diffusivity in silicon as a function of temperature and experiment. This large scatter in the data does not inspire confidence in the predictive ability of the simulator. Would anyone trust device simulators if we had controversy over four orders of magnitude regarding the carrier mobility? This is essentially the case for point-defect-based simulations.

Both point-defect types, interstitials and vacancies, cannot be measured directly and can only be measured indirectly through their effect on processes, e.g., diffusion. This leads to circular reasoning—there must be excess interstitials because phosphorus diffuses faster, and the reason for the faster diffusion of phosphorus is that there are excess interstitials present. Part of the scatter in the data is due to different interpretations of the measured result. This circular reasoning loop has resulted in controversy about the point-defect behavior in silicon.

V. THE NEED FOR DAMAGE PROFILING

The previous problems pale in comparison to the major challenge facing diffusion modeling, transient enhanced diffusion (TED). The diffusion of dopants is found to be enhanced at very short times and low temperatures. This is commonly thought to occur due to the damage from the implantation. The crystal damage is displaced atoms from lattice sites, interstitials, and vacancies. This large excess of defects is thought to enhance the diffusion until the damage completely anneals away. Since the defects cannot be directly measured, this initial defect concentration is a very difficult problem.

There have been some notable successes at modeling TED.[9–13] Unfortunately, most of this work has used different starting conditions for the defect profile after the anneal. Figure 4 indicates some of these models. The simplest approach is the plus one model, in which excess interstitials are assumed to be equal to the doping profile. The damage is assumed to be annealed instantly, and the dopant moves substitutionally and injects interstitials. The next approach is the net approach, where the vast majority of the defects are annealed instantly, leaving the difference in the vacancy and interstitial concentration behind. This results in a vacancy-rich region near the surface and an interstitially rich region deeper in the bulk. Finally, all of the damage reported by a Monte Carlo simulation can be used as the initial defect concentration. As might be expected, this results in a large discrepancy in the final extracted values of the dopant and defect parameters.

The next major problem is that the diffusion of dopants does not depend simply on the excess damage created by the implant. Generally, the diffusivity increase has a sublinear dependence on dose. For all the models proposed above, the damage density increases at minimum linearly with the implant dose. None of the current initial condition models can explain this phenomenon. There are two competing theories. The first suggests that the dopant becomes nearly completely paired with the defects, and further increases in the defect density do not increase the diffusion of the dopant.[9] The second suggests that the defects cluster into a stable phase, and then are slowly released to aid diffusion and recombine.[14] The second theory has received recent experimental support from AT&T,[15] where they have identified ⟨113⟩ defects that dissolve with similar time constants to that observed for enhanced diffusion.

One of the most interesting developments in characterization of diffusion processes has occurred over the last several years. Transmission electron microscopy has developed sufficiently to allow quantification of the interstitials bound in loops. The AT&T group is attempting to quantify the interstitials contained in the ⟨113⟩ loops as a function of time. This would allow verification of the interstitial release independent of a doping measurement, and provide information for modeling of TED. Kevin Jones has led a similar development in using end-of-range dislocations to getter intersti-

tials and provides quantitative information on the number of interstitials and vacancies released during various processes.[16] They have shown that the dislocation capture is diffusion limited,[17] and can therefore be used to measure the defect concentrations independent of a dopant.

VI. CONCLUSIONS

The accuracy of the simulators is determined by the models and metrology. It is extremely difficult to measure two-dimensional profiles, much less three. Model development, particularly phenomenological models that would be more computationally efficient, are slowed due to the lack of sophisticated measurement techniques. These two factors contribute to lack of motivation for development, since without accurate, verifiable models, multidimensional process simulators become ''garbage in, garbage out.''

All is not lost, however. There are bright spots on the horizon for two-dimensional measurement systems, some of which are being discussed at this conference. There have also been advances in measurement of point-defect behavior through phenomena other than dopant diffusion. Although unrelated to metrology, another bright spot is the first-principle molecular dynamics calculations that are planned at the National Labs, which may provide some additional insight.

ACKNOWLEDGMENTS

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[1]M. E. Law, *SISDEP Proceedings, Vienna, 1993*, edited by S. Selberherr, H. Stippel, and E. Strasser (Springer, Berlin, 1993), p. 1.
[2]R. Goosens and R. W. Dutton, IEEE Circ. Devices **8**, 18 (1993).
[3]A. M. Lin, R. W. Dutton, and D. A. Antoniadis, Appl. Phys. Lett. **35**, 799 (1979).
[4]C. Park, K. M. Klein, and A. F. Tasch, Solid-State Electron. **33**, 645 (1990).
[5]G. Hobler, E. Langer, and S. Selberherr, Solid-State Electron. **30**, 445 (1987).
[6]R. B. Fair, IEEE Trans. Electron. Devices **35**, 285 (1988).
[7]D. Mathiot and J. C. Pfister, J. Appl. Phys. **55**, 3518 (1984).
[8]M. Orlowski, Appl. Phys. Lett. **53**, 1323 (1988).
[9]H. Park and M. E. Law, J. Appl. Phys. **72**, 3431 (1992).
[10]M. D. Giles, J. Electrochem. Soc. **138**, 1160 (1991).
[11]P. B. Griffin, R. F. Lever, R. Y. S. Huang, H. W. Kennel, P. A. Packan, and J. D. Plummer, International Electron Devices Meeting, Washington, DC, 1993 (unpublished).
[12]C. S. Rafferty, H.-H. Vuong, S. A. Eshraghi, M. D. Giles, M. R. Pinto, and S. J. Hillenius, in Ref. 11.
[13]B. Baccus and E. Vandenbossche, International Electron Devices Meeting, San Francisco, 1994 (unpublished).
[14]P. A. Packan, Ph.D. thesis, Stanford University, 1991.
[15]D. J. Eaglesham, P. A. Stolk, H. J. Gossmann, and J. M. Poate, Appl. Phys. Lett. **65**, 2305 (1994).
[16]H. L. Meng, S. Prussin, M. E. Law, and K. S. Jones, J. Appl. Phys. **73**, 955 (1993).
[17]H. Park, H. Robinson, K. S. Jones, and M. E. Law, Appl. Phys. Lett. **65**, 436 (1994).