30 Years of Lithography Simulation

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ABSTRACT

Thirty years ago Rick Dill and his team at IBM published the first account of lithography simulation – the accurate description of semiconductor optical lithography by mathematical equations. Since then, lithography simulation has grown dramatically in importance in four important areas: as a research tool, as a development tool, as a manufacturing tool, and as a learning tool. In this paper, the history of lithography simulations is traced from its roots to today's indispensable tools for lithographic technology development. Along the way, an attempt will be made to define the true value of lithography simulation to the semiconductor industry.

Keywords: Lithography Modeling, History of Lithography Simulation, PROLITH

1. Introduction

Optical lithography modeling began in the early 1970s when Rick Dill and his team described the basic steps of the lithography process with mathematical equations. At a time when lithography was considered a true art, such an approach was met with much skepticism. The results of their pioneering work were published in a landmark series of papers in 1975 [1-4], now referred to as the "Dill papers." These papers not only gave birth to the field of lithography modeling, they represented the first serious attempt to describe lithography not as an art, but as a science. These papers presented a simple model for image formation with incoherent illumination, the first order kinetic "Dill model" of exposure, and an empirical model for development coupled with a cell algorithm for photoresist profile calculation. The Dill papers are still among the most referenced works in the body of lithography literature.

Thirty years later, optical lithography continues to make dramatic advances that enable the profitable continuation of Moore's Law. Most if not all of these advances would not be possible without the use of lithography simulators. This paper will review the history of lithography simulation, describing a few of the milestone events and important lithographic advances that simulation enabled. This historical review will end with a characterization of the current state of lithography modeling and a brief prediction of future advances in simulation capabilities.

2. The Need for Lithography Simulation

In the early days of semiconductor manufacturing, lithography was widely regarded as an art. The experienced lithographer, practiced in this art through on-the-job training, was able to deliver results but not always able to explain how or why. Processes were optimized (or at least made acceptable) through trial and error. Resolution limits were largely unexplored and feature sizes were many times larger than the wavelength of the light used. Even still, lithography was not easy and it often limited the successful manufacture of then state-of-the-art devices. Progress was made, but it was obvious that more could be done

with a more enlightened approach. As Larry Thompson noted as late as 1983, "... it is of paramount importance that we transform the important area of lithographic processing from an art to a science [5]."

The transformation of semiconductor lithography from art to science began in the early 1970s, and in my opinion is largely complete today. Mass production at very close to the (now well understood) theoretical limits of a given imaging technology is common. It is likely that 193nm wavelength imaging will produce sub-100nm pitch patterns in an amazing extension of optics to its extreme limits. The scientific approach to lithography is responsible for the amazing progress in resolution – beyond anyone's wildest predictions – that continues to enable Moore's Law. And at the very heart of this scientific makeover has been lithography simulation.

A philosophical diversion...

While the meaning and nature of science remains hotly debated among philosophers, practitioners of science follow a simple and clear approach to scientific advancement: science is the development of useful, predictive, and testable models that describe the behavior of the universe. These models (most often called theories, but often inappropriately labeled "laws" of nature) are almost always framed in the language of mathematics, with symbols representing physical quantities. A simple truism from this definition of science is that you cannot model what you don't understand. As the famous scientist William Thomson (Lord Kelvin) said, "Can you measure it? Can you express it in figures? Can you make a model of it? If not, your theory is apt to be based more upon imagination than upon knowledge." Quite simply, if you can't model an effect, chances are you don't understand it.

Lithography simulation is widely understood to be an essential tool for semiconductor lithography today. It is hard to imagine being able to design the next generation of lithography tools, materials, and processes without simulation to guide us. However, simulation has served an even more important though mostly unappreciated role in the development of lithography technology. As an industry, we use the development of lithography models as a tool to test and advance our understanding of lithography. Applying Lord Kelvin's admonition, we check our understanding of the underlying physics and chemistry of lithographic imaging by comparing the predictions of our models to experimental evidence. Ultimately, it is the advancement of our understanding of lithography that underpins all advances in lithography technology. And it is the advancement of lithography simulation that measures and informs our understanding of lithography.

3. Rick Dill and the Early Years

Optical lithography modeling began in the early 1970s when Rick Dill started an effort at IBM Yorktown Heights Research Center to describe the basic steps of the lithography process with mathematical equations [6]. Rick was frustrated with his ability to predict, or even intuit, the outcome of a lithographic experiment. Having come from a background in device physics where modeling was commonly used, he longed for similar scientific rigor to aid in his lithographic researches. But at a time when lithography was considered a true art, such an approach was met with much skepticism. Prompted by a high profile lithography-related "yield bust" at an IBM factory, he put together a team of talented researchers (Karl Konnerth, Peter Hauge, Jane Shaw, Jim Tuttle, Mitch Phillips, and Andy Neureuther who was on a one-year sabbatical from UC Berkeley) and started his now well-funded project.

Dill began by thinking about the modeling problem as simply as possible – in one dimension. Given an open-frame exposure of a photoresist film on an unpatterned wafer, what was the lithographic result as a function of depth into the resist? Dill first broke up the lithographic process into a sequence of needed

calculations: the intensity of light inside the resist (a calculation of the standing waves), the chemical concentration of exposure products resulting from this light, the impact of this chemistry on the development rate, and finally the integration of the development rate through time to predict the resist thickness after development. Fortuitously, Dill managed a parallel effort to develop an automated thin film thickness measurement tool and this technology proved essential for the development of his 1D lithography models.

By noticing that the diazo-type positive resists in use at the time "bleached" (become more transparent) upon exposure, Dill used this change in optical absorbance as a way of monitoring the kinetics of exposure. Coating the resist on an optically matched glass wafer, he measured the transmittance of the resist film as a function of exposure dose. The result was extremely well fit by a first order model of exposure, now called the Dill model. The three Dill parameters, called simply A, B, and C, described the bleachable and non-bleachable absorbance and the exposure rate constant, respectively.

The key to photoresist development modeling was the creation of a development rate monitor (DRM), a modified version of the thin film measurement tool IBM was soon to commercialize. This reflectance spectroscopy tool was customized to work through a fluid flow chamber surrounding the wafer. By measuring resist thickness in real time during development, development rate could be calculated as a function of depth into the resist. By repeating this measurement for many exposure doses, and using the Dill exposure model to relate incident dose to amount of chemical change within the resist, development rate as a function of the chemical composition of the resist was determined. Dill assumed that the development was surface rate limited and fit this data to a simple second order polynomial (on a log-development rate scale) to get his empirical development rate function. After measuring the development rate on a low-reflectance substrate, he confirmed the accuracy of his models by correctly predicting the depth dependent development rate of resist on a silicon wafer.

The pieces were now all in place. His 1D models accurately predicted the development rate as a function of depth into the resist. By combining these models with a simple incoherent imaging model and Andy Neureuther's cell algorithm for development, the first lithography simulator was created. The results of this pioneering work were published in a landmark series of papers in 1975 [1-4], now referred to as the "Dill papers." These papers not only gave birth to the field of lithography modeling, they represented the first serious attempt to describe lithography not as an art, but as a science. The Dill papers are still the most referenced works in the body of lithography literature.

4. The SAMPLE Years

While Dill's group worked on the beginnings of lithography simulation, a professor from the University of California at Berkeley, Andy Neureuther, spent a year on sabbatical working with Dill. Upon returning to Berkeley, Neureuther and another professor, Bill Oldham, started their own modeling effort. In 1979 they presented the first result of their effort, the lithography modeling program SAMPLE [7]. SAMPLE improved the state of the art in lithography modeling by adding partial coherence to the image calculations, adding a surface inhibition function to the development rate calculation, and replacing the cell algorithm for dissolution calculations with a string algorithm, which gave better results for larger grid sizes. But more importantly, SAMPLE was made available to the lithography community. For the first time, researchers in the field could use modeling as a tool to help understand and improve their lithography processes.

In the early years of the Berkeley modeling efforts, computers were slow and computer time was expensive (\$500/hour on a mainframe), and models remained relatively simple. As a sign in one of the researcher's office proclaimed, "We simulate yesterday's technology tomorrow." But despite the difficulties the effort gained momentum. For nearly 30 years (and still today), the SAMPLE research group at the

University of California at Berkeley has been one of the most important university efforts in lithography research. Using simulation as their research venue, the group has made numerous contributions to advances in lithography, including the first suggestion for the use of dyed photoresists, very early proposals for phase-shifting mask schemes, several resolution enhancement tricks, and the design of aberration sensitive monitor structures, among many, many other contributions. But undoubtedly, the most important contribution of the SAMPLE group was SAMPLE itself. Beginning in 1980, for a small fee, anyone in the semiconductor industry could receive a computer tape containing the SAMPLE code and (after compiling the code on their computer) begin using simulation to solve lithography problems. SAMPLE was written in Fortran and ran on mainframe computers (PC versions became available much later) using ASCII text "job decks" to control simulations. While not easy to use, simulating with SAMPLE was still easier than writing your own simulator, and SAMPLE grew in popularity among lithography R&D types. By the mid 1980s, simulation had a small but dedicated core following of people that recognized the need for using simulation when faced with the most complex lithography challenges.

5. The PROLITH Years

I began working in the field of lithography in 1983 at the National Security Agency. While trying to make sense of this difficult and interesting subject – when my boss first told me I was to practice lithography, I made her spell that for me – I ran across Rick Dill's 1975 papers. By the time I finished the last of the four papers I knew that lithography simulation would be my career. I had heard about SAMPLE and looked into getting a copy, but I didn't have convenient access to a mainframe computer. I had already become addicted to the new IBM PC on my desk, and decided that a "personal" simulator would be a good challenge.

After about one year I had finished a very early version of the PC software I called PROLITH, the Positive Resist Optical Lithography model. Building on the work of Dill and Neureuther and their teams, I derived an analytical expression for the standing wave intensity (rather than using the matrix calculation approach that Dill chose) and proposed a kinetic model for resist dissolution that later came to be called the Mack model. At this point the imaging calculation was a simple incoherent model, though I also developed a proximity/contact printing model since a contact printer was the only lithography tool then at my disposal. A chemistry lab allowed me to build ABC and development rate measurement capabilities and to characterize several resists.

This first simulation effort was published in 1985 after being presented at the SPIE Microlithography Symposium that year [8]. While I might judge the scientific aspects of this work to be of some value, it quickly become clear to me how the industry would judge my efforts. After mentioning at the end of my talk that I would give copies of PROLITH away free, 80 people handed me their business cards. The need for accurate simulation that could be conveniently used by everyday lithographers became obvious. For the next four years, the PROLITH software was updated (at taxpayer expense) to include contrast enhancement layers, partially coherent imaging, different approaches for extracting the dimension of a complex resist cross-section, and the "high NA" effect of image defocus through the thickness of the resist (Figure 1).

The continued interest and growing importance of PROLITH in the semiconductor industry prompted me to commercialize the software. FINLE Technologies was formed in February, 1990 and the first commercial version of what was now dubbed PROLITH/2 (the second generation of the PROLITH software) was released in June of that year. While still a DOS program, PROLITH began to take advantage of the improving graphics capabilities of the PC, as well as the gradual move towards graphical user interfaces (Figure 2a). By the end of the decade the inevitable switch to Windows had taken place (Figure 2b). While SUN and Macintosh versions of PROLITH were released, they proved uneconomical and were short-lived.

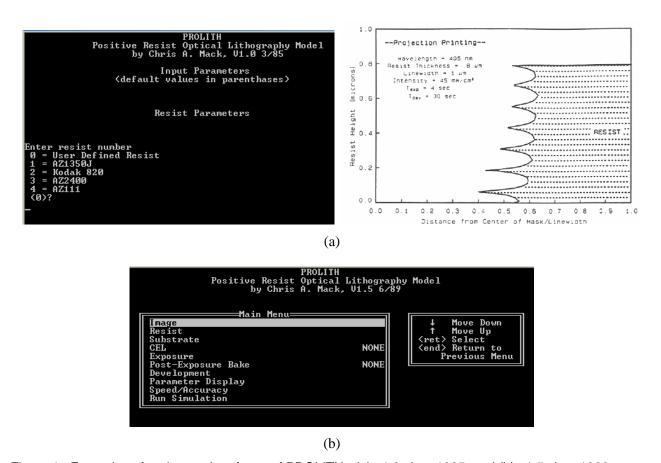


Figure 1. Examples of early user interfaces of PROLITH: (a) v1.0 circa 1985, and (b) v1.5 circa 1989.

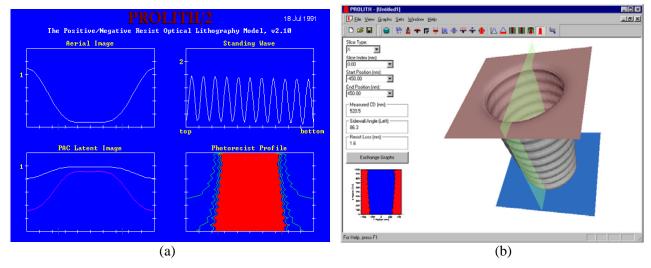


Figure 2. Examples of the user interfaces of the commercial version of PROLITH: (a) the DOS version 2.1, circa 1991, and (b) the Windows version 6.0, circa 1999.

Improvements in ease of use and convenience (automated generation of a focus-exposure matrix and process window, for example) were predictable consequences of commercialization, but the need for additional physics in the simulators led to significant developments in the core models. Here is a much abbreviated list and timeline of some of the new physics incorporated into PROLITH by the growing PROLITH team of researchers and developers:

- First chemically amplified resist model (v2.1 1991)
- Broadband illumination (v2.1 1991)
- Phase shift masks (v2.2 1992)
- Flex multiple focal plane exposures (v2.2 1992)
- Lumped Parameter Model, LPM (v2.2 1992)
- High NA Scalar model (v3.0 1993)
- Off-axis illumination (v3.0 1993)
- Vector imaging model (v4.0 1994)
- 2D masks and aerial images (v4.0 1994)
- Aberrations (v4.0 1994)
- Full 3D simulations (v5.0 1996)
- Variable diffusivity reaction-diffusion in 3D (v5.0 1996)
- Step-and-scan vibrations, scanner aberration averaging (v6.0 1998)
- Notch development model (v6.0 1998)
- Byers/Petersen chemically amplified resist model (v6.0 1998)
- AutoTune for calibration (v7.0 2001)
- 3D Lumped Parameter Model (v7.1 2001)
- Etch simulator (v7.2 2002)
- Base quencher diffusion (v7.2 2002)
- Immersion lithography (v8.0 2003)
- Mask topography EMF simulator (v8.1 2003)
- Birefringence (v8.1 2003)

In addition to improvements in accuracy, improvements in speed were regular and dramatic. In 1985 I ran my first focus-exposure simulation on eight borrowed PCs running overnight. Today, a much more accurate version of that simulation runs on a \$500 computer and finishes in under a minute. Of course, much of that has to do with hardware improvements. In the last 20 years, processor speed has increased from 4.77 MHz to 4GHz, processor architecture has shifted from 16 bit to 64 bit, and from multiple clock cycles per instruction to multiple instructions per clock cycle. Overall, there has been about a 10,000X improvement in hardware speed for a typical PC. In addition, the software has contributed another 500 – 1000X speed improvement due to better models/algorithms. This ten million-times improvement in speed, however, has been easily consumed by the users of lithography simulation. In 1985, simulations were two-dimensional, scalar, using conventional resists, and with low expectations for absolute accuracy. Today, 3D simulations of chemically amplified resists using vector calculations require one nanometer simulation uncertainty. And the uses of simulation have so greatly expanded that my crude distributed computing effort of 1985 is now automated on hundreds of PC blades to run thousands of simulation per minute.

PROLITH was not the only, nor even the first, commercial lithography simulator. Depict, originally based on SAMPLE, was developed by Bob Pack of Technology Modeling Associates and released for the SUN workstation in 1986. After a few acquisitions of the parent company, Depict eventually faded from the marketplace. Wolfgang Hencke of the Fraunhofer Institute developed the first 3D lithography simulator Solid in 1991, commercializing it the following year through a Silicon Valley company called Silvaco. After

the business relationship failed to meet Hencke's expectations, in 1994 Solid-C was released by the German company Sigma-C.

In February 2000, FINLE Technologies was acquired by KLA-Tencor. The PROLITH development team continues to work in Austin, Texas, with PROLITH v9.0 recently released.

6. The Impact of Lithography Simulation

In the 30 years since optical lithography modeling was first introduced to the semiconductor industry, it has gone from a research curiosity to an indispensable tool for research, development and manufacturing. There are numerous examples of how modeling has had a dramatic impact on the evolution of lithography technology, and many more ways in which it has subtly, but undeniably, influenced the daily routines of lithography professionals. There are four major uses for lithography simulation: 1) as a research tool, performing experiments that would be difficult or impossible to do any other way, 2) as a development tool, quickly evaluating options, optimizing processes, or saving time and money by reducing the number of experiments in the fab, 3) as a manufacturing tool, for troubleshooting process problems and determining optimum process settings, and 4) as a learning tool, to help provide a fundamental understanding of all aspects of the lithography process. These four applications of lithography simulation are not distinct – there is much overlap among these basic categories.

a. Research Tool

Since the initial introduction of lithography simulation in 1975, modeling has had a major impact on research efforts in lithography. Here are some early examples of how modeling has been used in research.

Modeling was used to suggest the use of dyed photoresist in the reduction of standing waves [9]. Experimental investigation into dyed resists didn't begin until 10 years later [10,11]. After phase-shifting masks were first introduced [12], modeling has proven to be indispensable in their study. Levenson used modeling extensively to understand the effects of phase masks [13]. One of the earliest studies of phaseshifting masks used modeling to calculate images for Levenson's original alternating phase mask, then showed how phase masks increased defect printability [14]. The same study used modeling to introduce the concept of the outrigger (or assist slot) phase mask. Since these early studies, modeling results have been presented in nearly every paper published on phase-shifting masks. Off-axis illumination was first introduced as a technique for improving resolution and depth of focus based on modeling studies [15]. Since then, this technique has received widespread attention and has been the focus of many more simulation and experimental efforts. Using modeling, the advantages of having a variable numerical aperture, variable partial coherence stepper were discussed [15,16]. Since then, all major stepper vendors have offered variable NA, variable coherence systems. Modeling remains a critical tool for optimizing the settings of these flexible machines. The use of pupil filters to enhance some aspects of lithographic performance have, to date, only been studied theoretically using lithographic models [17]. If such studies prove the usefulness of pupil filters, practical experimental investigations may also be developed.

Modeling has been used in photoresist studies to understand the depth of focus loss when printing contacts in negative resists [18], the reason for artificially high values of resist contrast when surface inhibition is present [19], the potential for exposure optimization to maximize process latitude [20,21], and the role of diffusion in chemically amplified resists [22]. Lithographic models are now standard tools for photoresist design and evaluation. Modeling has always been used as a tool for quantifying optical proximity effects and for defining algorithms for geometry dependent mask biasing [23,24]. Most people would consider modeling to be a required element of any optical proximity correction scheme. Defect printability

has always been a difficult problem to understand. The printability of a defect depends considerably on the imaging system and resist used, as well as the position of the defect relative to other patterns on the mask and the size and transmission properties of the defect. Modeling has proven itself a valuable and accurate tool for predicting the printability of defects [25,26]. Modeling has also been used to understand metrology of lithographic structures [27-30] and continues to find new application in virtually every aspect of lithographic research. In fact, modeling has proven an indispensable tool for predicting future lithographic performance and evaluating the theoretical capabilities and limitations of extensions for optical lithography far into the future.

One of the primary reasons that lithography modeling has become such a standard tool for research activities is the ability to simulate such a wide range of lithographic conditions. While laboratory experiments are limited to the equipment and materials on hand (a particular wavelength and numerical aperture of the stepper, a given photoresist or film stack), simulation gives an almost infinite array of possible conditions. From high numerical apertures to low wavelengths, hypothetical resists to arbitrary mask structures, simulation offers the ability to run "experiments" on steppers that don't exist with photoresists that have yet to be made. How else can one explore the shadowy boundary between the possible and the impossible?

b. Process Development Tool

Lithography modeling has also proven to be an invaluable tool for the development of new lithographic processes or equipment. Some of the more common uses include the optimization of dye loadings in photoresist [31,32], simulation of substrate reflectivity [33,34], the applicability and optimization of top and bottom antireflection coatings [35,36], and simulation of the effect of bandwidth on swing curve amplitude [37,38]. In addition, simulation has been used to help understand the use of thick resists for thin film head manufacture [39] as well as other non-semiconductor applications. Modeling is used extensively by makers of photoresist to evaluate new formulations [40,41] and to determine adequate measures of photoresist performance for quality control purposes [42]. Resist users often employ modeling as an aid for new resist evaluations. On the exposure tool side, modeling has become an indispensable part of the optimization of the numerical aperture and partial coherence of a stepper [43-45] and in the understanding of the print bias between dense and isolated lines [46]. The use of optical proximity correction software requires rules on how to perform the corrections, which are often generated with the help of lithography simulation [47], or they use lithography models directly for the corrections.

As a development tool, lithography simulation excels due to its speed and cost-effectiveness. Process development usually involves running numerous experiments to determine optimum process conditions, shake out possible problems, determine sensitivity to variables, and write specification limits on the inputs and outputs of the process. These activities tend to be both time consuming and costly. Modeling offers a way to supplement laboratory experiments with simulation experiments to speed up this process and reduce costs. Considering that a single experimental run in a wafer fabrication facility can take from hours to days, the speed advantage of simulation is considerable. This allows a greater number of simulations than would be practical (or even possible) in the fab.

c. Manufacturing Tool

Although you will find less published material on the use of lithography simulation in manufacturing environments [48-50], the reason is most likely the limited publications by people in manufacturing rather than the limited use of lithography modeling. The use of simulation in a manufacturing environment has three primary goals: to reduce the number of test or experimental wafers which must be run through the

production line, to troubleshoot problems in the fab, and to aid in decision making by providing facts to support engineering judgment and intuition. Running test wafers through a manufacturing line is costly not so much due to the cost of the test, but due to the opportunity cost of not running product [51]. If simulation can reduce the time a manufacturing line is not running product even slightly, the return on investment can be significant. Simulation can also aid in the time required to bring a new process on-line and in the establishment of the base-line capability of a new process. Although not a complete list, the most common use cases for lithography simulation in a manufacturing environment are:

- Film Stack Optimization
- Process Window Prediction
- NA/σ optimization
- OPC Verification
- CD Limited Yield, Cpk Analysis
- Troubleshooting/Root Cause Analysis

d. Learning Tool

Although the research, development and manufacturing applications of lithography simulation presented above give ample benefits of modeling based on time, cost and capability, the underlying power of simulation is its ability to act as a learning tool. Proper application of modeling allows the user to learn efficiently and effectively. There are many reasons why this is true. First, the speed of simulation versus experimentation makes feedback much more timely. Since learning is a cycle (an idea, an experiment, a measurement, then comparison back to the original idea), faster feedback allows for more cycles of learning. Since simulation is very inexpensive, there are fewer inhibitions and more opportunities to explore ideas. And, as the research application has shown us, there are fewer physical constraints on what "experiments" can be performed. In addition, simulation allows one to "see" intermediate parts of the imaging sequence, like aerial images, latent images, and substrate reflectivity, that are not observable in practice. All of these factors allow the use of modeling to gain an understanding of lithography. Whether learning fundamental concepts or exploring subtle nuances, the value of improved knowledge cannot be overstated.

The list above is, by necessity, extremely incomplete. It is also quite dated. While it was easy in the early years of the history of simulation to identify milestone papers that illustrated the importance of simulation to the four use cases described above, today it is much more difficult. Simulation is so well ingrained into the working world of the lithographer today that it is difficult to single out any small handful of papers as being significant above the rest in their use of simulation.

7. Conclusions and the Future of Lithography Simulation

Lithography simulation has for 30 years served two essential purposes: to validate and improve the industry's theoretical understanding of lithography, and to provide a tool to the average lithographer to apply this theory to real lithography problems. By both of these measures, the industry's efforts in lithography simulation have been extremely successful. It is not an overstatement to say that semiconductor manufacturing as we know it today would not be possible without lithography simulation.

But just as lithography technology moves at a harried pace toward finer features, simulation technology must move just as fast to stay with, or ahead of, the needs of lithography technology development. The future of simulation will be even more challenging than the past has been – but success is a requirement. There are three major areas of lithography simulation development for the foreseeable future.

a. Accuracy

Lithographers want simulation to be more accurate than their experimental data. While this goal may seem unattainable, in fact it is quite possible. For example, a requirement for a lithography simulator might be a Total Simulation Uncertainty (TSU) of less than 2nm at the 65nm node. Much, probably most, of the focus of model and simulator development today is on achieving greater accuracy.

b. Full chip simulations

Today, full chip lithographic simulation using approximate image models and empirical resist models has enabled useful optical proximity correction (OPC) technology. These models, however, show reduced accuracy compared to full physical models (3X - 10X less accuracy) over a much narrower range of process conditions as the price paid for sufficient speed to make a full chip simulation practical. There is, then, a need for even faster simulations with more physically-based models that provide much better accuracy over a wider range of process conditions for a single calibration. Research efforts along these lines will undoubtedly make design for manufacturing (DFM) more than just an industry buzzword.

c. Mesoscale Modeling

An interesting effort at several universities (the University of Texas at Austin being predominate) involves so-called mesoscale modeling, working down at the molecular level for its physical descriptions. While much work remains to be done, mesoscale modeling efforts could one day aid in resist design and provide invaluable insight into the mechanisms of line-edge roughness formation and statistical feature size fluctuations.

The remarkable successes of lithography simulation reflect the broader successes of lithography technology development and semiconductor manufacturing advancement. And just as the continued improvements in resolution and manufacturability in our industry seem inevitable, so too will lithography simulation development continue and advance.

8. Acknowledgements

I would like to thank Rick Dill and Andy Neureuther for sharing their experiences and memories with me. I only wish that I had the time and space to include more of their anecdotes and histories in this work.

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