# Simulating Process Subtleties in SEM Imaging 

Benjamin D. Bunday ${ }^{\text {a }}$, Shari Klotzkin ${ }^{\text {b }}$, Douglas Patriarche ${ }^{\mathrm{c}}$, Maseeh Mukhtar ${ }^{\text {d }}$, Kotoro Maruyama ${ }^{\text {e }}$, Seul-Ki Kang ${ }^{\text {e }}$, Yuichiro Yamazaki ${ }^{\text {e }}$<br>${ }^{a}$ aMAG Consulting, LLC, Schenectady, NY, 12303, USA; e-mail: benbunday @amag-consulting.com<br>${ }^{\text {b }}$ AMAG Consulting, LLC, Binghamton, NY, 13850, USA<br>${ }^{\text {c AMAG Consulting, LLC, Ottawa, ON, K2G 5M9, Canada }}$<br>${ }^{\mathrm{d}}$ KLA, Milpitas, CA, 95035 , USA<br>${ }^{\text {e}}$ TASMIT/TORAY Inc., Yokohama-shi, Kanagawa-ken, Japan 222-0033


#### Abstract

Microscopically, a rough surface (or any other feature) can be considered as a set of perturbations from the idealized surface. In reality, the microstructure of such a roughness may include spatial components some being smaller (subresolution) and some larger spatial frequency than the spot size of the SEM, and this should affect SE yields from such a target with respect to an ideal smooth surface. Yet to explore such influences by simulation, Monte Carlo SEM simulations are necessary but quite resource hungry, and thus somewhat limited in ability to include much fine detail, and with SEM simulation codes still being developed to include such effects easily, until now we typically simulate perfect smooth idealized structures. Other examples of such simulation resource-limited simplification of features could be etch halos at base of an etched feature, pits, bumps, craters, scratches or defects on or below the surface, CMP dishing, top corner rounding or footing at the base of a resist line or contact hole, or many other possibilities. We know these will add signatures to the simulated image, but it is important to understand how important are they to achieving realistic results.


In this work, several different cases of such process subtleties from the above list of examples will be simulated and compared to results from simulated idealized features, to determine the significance of such details compared to typical noise. More complex features can now be modeled using NIST's JMONSEL [1-16] through a new improved version, AMAG SimuSEM, which essentially completes SEMATECH AMAG's original vision for JMONSEL by adding a powerful GUI, and updates the software to current expectations by greatly improving utility, productivity, flexibility, visualization, accessibility, and achievable complexity of designed features while improving simulation speed and allowing user to run on remote resources at larger scale. Additionally, the new code allows viewing of all electron trajectories in the 3D environment which allows additional observations on how various process subtleties might affect the SEM signal. The work will conclude with how some of these subtleties might influence accuracy.

Keywords: SEM, CD-SEM, DI-SEM, JMONSEL, roughness, dishing, footing, defect, Monte Carlo simulation

## INTRODUCTION

Monte Carlo SEM simulations are necessary but resource hungry, thus usually include few fine details. Perfect smooth idealized structures are the norm. Other subtleties of interest include defects such as pits, bumps, etch halos, sidewall bowing, craters, scratches or defects on or voids or particles below the surface, CMP or etch dishing, top corner rounding or footing at the base of a resist line or contact hole, or many other possibilities. We know these will add signatures to the simulated image, but it is important to understand how important are they to achieving realistic results.

In this work, several different cases of such process subtleties will be simulated and compared to results from simulated idealized features, to determine the significance of such details compared to typical noise. More complex features can now be modeled using NIST's JMONSEL through a new improved version, AMAG SimuSEM, which essentially completes SEMATECH AMAG's original vision for JMONSEL by adding a powerful GUI, and updates the software to current expectations by greatly improving utility, productivity, flexibility, visualization, accessibility, and achievable complexity of designed features while greatly improving simulation speed and scalability. Additionally, the new
software allows viewing of all electron trajectories in the 3D environment which allows additional observations on how various process subtleties might affect the SEM signal.

## IMPORTANCE OF SEM SIMULATIONS

To fabricate in the nanoscopic size regime, one must be able to competently image and measure what is being built. Thus, the importance of improved metrology continues to grow as Moore's Law progresses and devices continue to shrink, become more complex with multiple layers and new include materials. Scanning Electron Microscopes (SEMs) image physical samples using scanning electron beams - electrons raster across solid objects and collect intensity/energy versus position information to form maps showing surface structure with possibly some depth information measuring backscattered electron yields.

SEM measurements are crucial in R\&D and manufacturing of semiconductor chips. However, these types of measurements are very expensive, and simulation support helps chip manufacturers achieve measurements that improve manufacturing yield, are statistically significant enough to make process decisions, and save time and money accelerating development of next generation chips. SEM simulation capability will contribute to the metrology understanding necessary during IC device fabrication, both during development of new devices and manufacturing process control. The tightness of the distribution of widths of billions of transistors on a chip is only producible to tolerance with the appropriate process monitoring.

SEM metrology is the main workhorse technique for a fab's process control, and a fab's eyes to yield-killing defectivity. These tools are operating near resolution and speed limits, such that simulation support for understanding the measurements and images is critical to successful, constructive and stable metrology. SEM imaging and electron beam condition optimization is important for achieving the best signal to noise possible of the aspect of the feature under evaluation, and this optimum is very sample-type and condition dependent. Additionally, if exploring items not easy to build at time of interest, as is the case when process development begins, simulation is an inexpensive alternative to tailor-building tools to explore a trial condition, or have built to perfection applicable samples for physical imaging case studies, samples which might be items possible years in future which cannot be built very well at the time a preliminary study is needed. Simulation allows conclusive results for such studies due to the full knowledge of the user-defined sample, and at a very small fraction of the cost or time involved for physical experiments. Once validated, a SEM simulation model can be used to extrapolate similar imaging to mass produce images over an entire process window, which can be effective for dealing with models involving larger parameter spaces. Simulation thus allows predictions to target other efforts, along with other advantages such as tailored model-based algorithms to measure a given case of interest, which will be necessary to maintain accurate and precise measurements of features of sizes close to resolution limits at 5 nm and 3 nm nodes and beyond. Also, such simulations can be used to produce images for other purposes such as calibrating AI image analysis tools with faux images, studying the evolution of 2D shape contours of different features at different conditions, or for providing a standard for comparison to other metrologies thru physical data or comparison of simulation results. Also, SEM simulations are used to determine best SEM conditions for measurement or imaging of various applications, or understand issues in measuring various feature types. Recently, the advent of HVSEM becoming mainstream fab tools has enabled ability to calibrate optical overlay with see-through SEM imaging, and simulators are valuable for understanding needed beam conditions to detect desired buried signals for different applications. SEM simulation is crucial for understanding the SEM metrology best practices, conditions and error sources which influence the success of metrology in such efforts.

## NIST JMONSEL \& AMAG SimuSEM

Such SEM simulators have been available for a while. JMONSEL, Java MONte Carlo Simulator for Secondary Electrons, is a 3D electron beam simulation software package developed and programmed in the 2010-12 timeframe at National Institute of Standards \& Technology (NIST) by Dr. John Villarrubia using Java/JYTHON, funded by SEMATECH AMAG to enable limits simulation studies for defect and critical dimension SEM metrology. NIST has supported ongoing improvement and validation efforts since, and it is now well validated for non-charging cases, with some use by a small user community.[1-16]

JMONSEL uses finite element analysis (FEA) to track primary electrons as they enter a material, scatter, lose energy, and generate secondary \& backscattered electrons. By monitoring the electrons that exit the material and are captured by a detector (software counter element), the electron yields can be found at any point designated as a target pixel. The physical models in JMONSEL are the best-known models in the literature in the energy ranges used here, open-source, with complete transparency in their documentation, definition, implementation and execution, as programmed by NIST, with a decade of validation data and wide acceptance by the industry.

However, the primitive JMONSEL code does have shortcomings. The largest of these is lack of user-friendliness; gaining proficiency with the primitive JMONSEL code takes much time with a steep and long learning curve, and the sample definition functions, while simple at a basic level, can become extremely complex to visualize for the programmer when trying to design features of the complexity of modern-day device structures or any 3D shapes beyond a few basic included shape primitives, impractical to code on a large scale for complex features. It had only minimal visualization thru VRML viewed in a web

```
Layer.s3
    location = [ 0.000*meterspernm, 0.000*meterspernm,557.500*meterspernm}
    otation = [ 0.000*math.pi, 0.000*math.pi, 0.000*math.pi]
    dimensions = [500.000*meterspernm,500.000*meterspernm, 15.000*meterspernm]
    thickness3=1ocation[2]+dimensions[2]/2
    layers3-mon.NormalMultiPlaneShape()
    layers3.addPlane (normalVector, [0,0,thickness2])
    layers3.rotate(location,-math.pi/2,rotation[0],math.pi/2)
    layers3.rotate (location,0, rotation[1], rotation[2])
    layers3region = monte.addSubRegion(layers2region,SiMSMDeep,layers3)
```

Figure 1: example few lines for describing a feature in a conventional preSimuSEM JMONSEL script which can be as long as 1000 lines of rigorous math and spatial relationships, with no means for visualization of the target other than trial and error which is very cumbersome and timeconsuming, and with the extreme detail involved complex features are very challenging to define, if not practically impossible. browser, no graphical interface. Original JMONSEL required very rigorous, involved, detailed line-edited Jython scripts, that typically would be 600-1000 lines long or more, and were themselves full Jython programs that called up core JMONSEL functions. See Figure 1 of a small part of a Jython script to just define part of the substrate.

Another shortcoming of original JMONSEL was that it was not speed optimized; small images would take hours, and large projects could take days or months, especially when charging was attempted which ran so slow were deemed impractical. Old JMONSEL had issues with sometimes pixel times increasing with number of pixels such that larger jobs would gradually bog down and take very long to finish near the end.

To fully modernize JMONSEL and make it practical and very useful in current times, AMAG Consulting is developing a software package called SimuSEM, which uses JMONSEL as its core physics but addresses JMONSEL's shortcomings by greatly improving the simulation run speed and providing a user-friendly front-end GUI and tools to visualize and analyze the results. SimuSEM, which includes many original improvements to JMONSEL, is a modern intuitive 3D graphical GUI which makes the code much more usable, with JMONSEL's runtime speed issues also addressed. This program provides the user with greatly improved utility, productivity, flexibility, visualization, accessibility, and achievable complexity of designed features while improving simulation speed and scalability, plus many other refinements and additions, and superior results access. Additionally, the new code allows viewing of all electron trajectories in the 3D environment and other nanoscopic views of the results. Thus, additional observations on how various process subtleties might affect the SEM signal can be studied. See Figure 2 for comparison to Figure 1 to see how all JMONSEL functionality is now built into Blender.[24] The improvement in simplification for the user, utility and visualization is obvious. All features are now reduced to best practices based on much experience using the code by the authors, who have built the SimuSEM GUI with accessibility to features and sample and results visualization as priorities

Speed optimization of JMONSEL also got a major overhaul as a major targeted improvement, so in this project these issues have been addressed and the runtime simulation speed optimized $>35 \mathrm{x}$ for a single core but with multithreading added, >200x faster than original JMONSEL with confirmed unchanged outputs, and with the pixel time slowdown issue eliminated.

AMAG SimuSEM's GUI is realized by building all the core JMONSEL code for writing runnable JMONSEL simulation scripts directly into a contemporary widely-acclaimed open-source 3D modelling and graphics engine, Blender, along with GMSH mesh generation program. Blender is a flexible platform with very powerful game-quality graphics engine that is used in the entertainment industry such as for Cartoon Network animations and to design 3D shapes for 3D
printing, but is also actually a very effective 3D Cartesian space object workbench which has recently been discovered by the scientific community as a way to create excellent geometries needed for 3D simulations. Blender is a great fit with JMONSEL as it supports Python addons, allowing JMONSEL to be directly incorporated and the interface customized to the application.[21] A Python program is being developed to customize JMONSEL into Blender's GUI to create a bridge between Blender and JMONSEL. The result is a 3D sample designing environment with definable virtual SEM functionality. Additional Python modules are installed to provide other functionality, including analysis and plots of simulation results viewable alongside Blender's 3D model. GMSH has a Python API to allow grid generation to be accessed through the customized GUI. By combining these programs, functionality that is already available does not need to be recreated and is standardized for common use.


Figure 2: example AMAG SimuSEM intuitive sample definition window for same sample as above (all $\sim 1000$ lines of script automatically produced for this shown sample by this constructor), which allows full 3D visualization at any scale or angle including see-thru mode, a good set of ready-to-use shape types, simple mouse-driven modification and many best JMONSEL practices and features plus new features with SimuSEM, with all routines built into a systematic package making all capabilities commonly available and ready for user deployment.

JMONSEL does have a charging model which is theoretically quite sound, but the past JMONSEL speed issues mean it has not been tested much and remains mostly unused in typical work. With the new speed improvements, charging will become a usable feature in SimuSEM. Another shortcoming was the moderate materials library, and the project also has plans in the works to improve that situation.

SimuSEM includes a large evolving list of shape primitives, all of which can be translated, rotated, scaled and defined parametrically but also with manual GUI manipulation by mouse. The user uses these and other constructions within the GUI to easily construct sophisticated target designs and control the scanning regions with full control of beam parameters and pixel locations. Pixel locations are all directly viewable, and great care has been taken to confirm what shows in the Blender GUI window is exactly what is achieved in JMONSEL. Figure 3 shows many translation/rotation matrices tested to confirm that fidelity for each primitive type, through various defined translations and rotations around each axis.


Figure 3: Translation/rotation matrices for testing many of the shape primitives in AMAG SimuSEM.
Addressing the lack of 3D visualization of the user's design with a modern GUI is important for the user to achieve applicable designs with complexity and detail. SimuSEM adds this all-important 3D visualization to JMONSEL. As a result, the complexity of the samples that can be created for a JMONSEL simulation without the GUI is extremely limited, and the time taken for a user to develop a complex or even simple design is much longer due to this lack of
visualization. The core JMONSEL code has been validated over the last ten years and works well for the electron material interactions, however JMONSEL has sorely lacked a GUI front end that makes such a simulator much more usable and powerful. Adding the intuitive GUI and other improvements to JMONSEL, AMAG SimuSEM is the greatly accelerated, user-friendly, mature version of JMONSEL with rich and reliable visualization, with the scripting handled automatically, allowing even users with minimal SEM experience to transparently unlock this powerful code through the greatly improved interface. With the script rigor removed, JMONSEL, thru AMAG SimuSEM, is now modernized to address many more simulation cases with much more complexity as required for contemporary needs. Figure 4 shows some more example images of achievable complex features.


Figure 4: Image gallery showing achievable complexity of features in SimuSEM.

## VIRTUAL EXPERIMENTS

The goal of this simulation study is to simulate process details and subtleties and evaluate their significance in terms of SNR. Much previous work has been done with JMONSEL and other SEM simulation software, but using more primitive block features. SimuSEM allows more complexity so we will explore several cases that were impractical before. Combining the above features enables studying subtleties with more realistic defects, rough surfaces and facets, photoresist footing, CMP, etch dishing, haloing, and detailed profile shapes, for some examples as shown in Figure 5. These include:

- Realistic defect types
- Rough surfaces \& facets
- Resist footing
- CMP/etch Dishing/haloing
- Detailed profile shapes


CMP/etch Dishing/haloing

b)

https://www.researchgate.net/figure/Conc eptual-framework-showing-dishing-and-erosion-after-barrier-CMP-as-referred-to-inthis fig2 270602792

Figure 5: General cases explored in this study.

## INTENTIONAL DEFECT ARRAY BY EBI

Past studies of EBI-SEM using JMONSEL are available in the literature.[11-13][15-16] To demonstrate how much more detailed intentional defect array (IDA) studies can get, a large test cell was designed within 2-3 hours in SimuSEM. The IDA consists of 10 nm wide Si links at 30 nm pitch, and includes holes, pits, craters, different particles of different shapes and materials, sub-surface voids/materials, mousebites and undercut link, missing link, extensions and protrusions. The image was simulated at $500 \mathrm{~V}, 1000 \mathrm{~V}$ and 2000 V beam energies with a $1 \sigma=2 \mathrm{~nm}$ beam with 3 nm pixels and $\mathrm{N}=30$ electrons per pixel per frame with 10 frames collected. The fins and substrate are all Si (gray), and green items are copper, light blue is $\mathrm{SiO}_{2}$, hot pink is tungsten, brown is PMMA, and the black meshed shapes are vacuum Boolean subtractors to leave holes, pits, mousebites, etc.


Figure 6: Intentional Defect Array (IDA) as viewed in SimuSEM from different aspects and with X-ray vision mode example for seeing buried features, and also showing how the image can not only be viewed conventionally from topdown but also directly viewed exactly over appropriate topography in the 3D view.

Analysis of signal versus background can give certainty of detection $\sigma_{\text {diff }}$ for different conditions for different defects to see what is detectible at various dose levels. In general, at $\mathrm{N}=30$, only gross defects are detectible. At $\mathrm{N}=100$, the smaller holes and most heavier particles seems to be detectible. At $\mathrm{N}=300$, most of the surface defects show, and at $\mathrm{N}=1000$ most defect types show with high certainty, although Si defects are still difficult to detect. Such SNR results are shown below.


Figure 7: Top Left: Plan view of sample. Top Right: Plan view of simulated image at 500 V and $\mathrm{N}=30$. New 3D views such as raytracing image onto sample surface will enable far superior visualization, coming soon in SimuSEM using Blender's superior graphics capabilities. Bottom Left: Plan view of simulated image at 500 V and $\mathrm{N}=90$. Bottom Right: Plan view of simulated image at 500 V and $\mathrm{N}=300$.

Images such as above underwent an analysis of all the various defects compared to background to estimate SNR for each defect for each beam voltage at various doses to understand how detectible they are, and demonstrating this with more realistic defect structures than in the past, although this is a single study and did not systematically explore the entire space. Results for the extreme doses of $\mathrm{N}=30$ and $\mathrm{N}=1000$ are shown below where different defect types become detectible at an assumed $1 \sigma$ yield contrast. Notice BSE's with 2000 V detect the buried defects, they become apparent at $\mathrm{N}=100$.


Figure 8: SNR results of all IDA defect types in sample for different simulated beam energies, for two different electron doses. Most defects do show at least one imaging solution where the defect is more than $1 \sigma$ above noise.

## ROUGH LINE SEGMENT

Stochastic issues such as roughness are uncertainty sources and prevalent limits to capability in the age of EUV patterning, thus accurate roughness measurement is a hot topic in the metrology community [10], and has for a long
time.[25][26] Roughness measurement of photoresist features involves a complex interplay among multiple components, including the stochastic roughness of the feature edge all the way up the profile, the profile shape including possibly stochastic shape, stochastic beam spot interacting with the sidewall, charging of the material [17], and photoresist shrinkage due to interaction of the beam with the polymeric photoresist material.[18-23] Understanding how each component effects accuracy is difficult to achieve experimentally yet much simpler with simulations since user defines the measurands and can define the various components individually, thus knows the answer the metrology should give beforehand.

SimuSEM includes ability to define normal height shape maps (NHSM's) as z-height maps of a pixelated structure which can be either defined by user or randomly generated for random surface roughness of a facet. Combining these with other features in the code allows definition of rough line segments, and what is shown here is just the prototype, better and automated version are in development. See figure 9 below, an NHSM is applied to sidewall of a trapezoidal line segment to achieve a rough line segment.


Figure 9: Rough PMMA line segment prototype for simulating a key stochastic case of interest. Left: plan view of design. Center: top view with perspective. Right: sideview showing profile. The brown straight edge on the right of the feature is the added foot with triangular cross section and 2 nm height.

The structure was defined as PMMA (brown) on Si (gray) and the right sidewall has an added PMMA foot 2 nm tall and extending out as a triangular wedge on Si surface a few nm out from feature. Figure 10 shows simulated results from the rough line edge in figure 9 , at 500 V beam energy, $\mathrm{N}=100$ per frame with 10 frames total, and with 0.5 nm square pixels.


Two important observations can be made from the results. First, the upper left and lower right (UL \& LR) edge minima show narrow ridges along edge in y direction closer into profile as shown in Figures 10a and 10b. In 10c those feet are hard to discern from noise. They seem to scatter less and base gets difficult to see, closer to noise limit. So profile shape issues up the line can in some parts of the structure effect what is seen at the profile bottom edge. With enough dose as in

Figure 10d, they are more apparent. However, remember that low dose is usually a necessity so that photoresist shrinkage is not as large a component influencing the measured roughness value.

The second key observation that can be made from these results is that the PMMA foot is not observed to any degree, at neither $\mathrm{N}=100$ or $\mathrm{N}=1000$ doses. For many years most have assumed a triangular-cross-sectioned foot was present and is usually $\sim 2 \mathrm{~nm}$ high, it is often seen in XSEM, however these results are interesting in that they imply we cannot detect such a foot from topdown imaging at 500 V in the dose regime we typically use. Thus, a DOE of foot size detectability is of interest.

## PHOTORESIST FOOTING

To look specifically at the signal from photoresist footing, a PMMA (brown) trapezoidal line structure with feet along 10 nm segments of the run of the line are added as triangular wedges of various heights ranging from 1 nm to 5 nm in 0.5 nm increments, and also portions of the line had no foot as a standard for comparison. Substrate is Si (gray). The resulting simulation was run at $\mathrm{N}=100,500 \mathrm{~V}$ beam and half nm pixels to see the differences in linescans among the different cases. Figure 11 shows the structure and Figure 12 the linescans/waveforms around the base of the feature.


At $\mathrm{N}=100$ the $1 \sigma$ noise of the background is $\sim 0.12$. SE signal difference between different steps of footing thus is well within $1 \sigma$ of noise from background, so if the background includes noise, it will make detection challenging, and even without more background these results imply a 3 nm foot or higher is more likely detected but 2 nm foot is likely difficult to detect.


Figure 12: Results from DOE of photoresist footing response. Left: waveform of full line segment with different curves for different foot heights in nm . Right: close-up on segment of results near edge of interest, showing low confidence in ability to discern among results from different foot heights below 3 nm .

## CMP DISHING

Chemical Mechanical Polishing (CMP) often leaves structural artifacts and defectivity in the form of dishing of damascene copper line (green in figure) surface or a more broad dishing of the $\mathrm{SiO}_{2}$ oxide (light blue in figure) over an entire grating pad. Typically, OCD or AFM are used to monitor and evaluate such issues, and SEM is not conventionally thought to be a good candidate for this application, however a simulator can be used to explore this use case to see if any


Figure 13: CMP test cell with multiple types of CMP dishing included, as marked.
capability is there, and surprisingly there might be some model based solutions made possible from such efforts, as significant signals can be observed. Figure 13 shows a CMP test cell that tests multiple types of dishing (and flat version


Figure 14: CMP dishing results.
as control feature) as a quick survey to check signals. The copper lines (green) in front have different amounts of dishing in terms of ratio of height of the curvature to width of the line, $10 \%, 20 \%, 30 \%, 40 \% 50 \%$ and $100 \%$ for the six copper lines left-to-right. The other dishing types were not studied parametrically through multiple steps, but could be in a more detailed future study. However broad trends are visible as seen in Figure 14, with signals far exceeding expected background noise levels. Beam energy is 800 V , with 0.5 nm pixels and $\mathrm{N}=1000$ as higher dose is not an issue for such samples so realistically would be used to suppress noise if measured in a production environment.

CMP results are shown in Figure 14. Large signatures can be observed with Cu dishing (well above noise), although seems not much variation depending on how much dishing in range tested, and if so, beneath noise. Future work will be to test more subtle amounts of dishing, covering that range under $10 \%$, as somewhere in that range the signal should transition from the signal from the flat regions to the one shown at $10 \%$ dishing. Oxide dishing appears less sensitive, although peaks emerge at grating edges if dishing is present. Thus, a model-based solution for that application might be promising. When oxide and Cu dishing are both present, large changes in contrast appear. A model-based solution is likely possible for this case as well, more exploration would be needed. Lastly, one type of dishing included discontinuities at the edge of the copper being recessed 2 nm below the oxide lip, and that discontinuity seems to suppress the peak at edge of Cu .

So, very ample signal responses exist for such a non-conventional SEM application as CMP dishing monitoring; more experiments by simulator through a much more exhaustive DOE could give much insight as to what the responses are and how they scale with the parameterized inputs to the structure.

## HAR HOLES

A last case to be looked at in this preliminary study is HAR (high aspect ratio) contact holes. Figure 15 shows such a hole feature, using AMAG7 reticle patterned to 60 nm holes with 120 nm pitch and etched into $1 \mu \mathrm{~m}$ deep $\mathrm{SiO}_{2}$ with a Si bottom. These same holes are simulated as lum deep truncated cones of vacuum cut out of a $1 \mu \mathrm{~m}$ thick $\mathrm{SiO}_{2}$ layer on top of Si substrate, with 70 nm top diameter and 50 nm bottom diameter. Various beam energies from 500 V up to 30 kV were used, with 1 nm pixels and $\mathrm{N}=1000$ dose. Each hole received a radial scan from outside hole to hole center to check trajectories at key points at top of sidewall, middle of sidewall and hole bottom, and the waveforms also are of interest in checking for signs of the known edge at hole bottom.


Figure 15: HAR hole features. Patterned using AMAG7, with 60 nm top CD and 50 nm bottom CD and 1000 nm depth. The image on right is topdown CD-SEM image at 800 V beam and 660 nm FOV. The image in center is XSEM showing depth of $1.03 \mu \mathrm{~m}$. On right is SimuSEM simulated image of center 4 holes in a $4 x 4$ array, scaled to match lefthand topdown experimental image, showing same basic yields and contrast, although the profile of the simulated features will need to be made more precisely to the real achieved profiles and charging included in the simulation to get a better match.

In SEM imaging cases such as these deep holes, views of the electron trajectories can be viewed qualitatively for much understanding of what scattering is important from given features at different locations within the features. Figure 16 shows 3D views of different such cases within the HAR holes at 800 V beam, from sideview and in Figure 17 also down the hole in 3D, and even from the aspect of underneath the hole.



Figure 16: 3D trajectory plots of 800 V electrons in 1000 nm deep HAR holes, for case of beam hitting top corner of hole, halfway down sidewall of hole, and bottom of hole. Not much returns from hole bottom but this can be observed with these views, along with the typical interactions in this imaging with most of the interaction volume staying near the point and few electrons escaping at 800 V .


Figure 17: 3D views of electron trajectories of hits at hole bottom from (right) top view and (left) from underneath the hole.
Additionally, 2D views of all of the electron trajectories at all the beam voltages for the pixel in middle of the sidewall are shown in Figure 18. These views show the extent of the interaction volume well and give a full display of the nature of the escaping electrons for many different beam energies attempted.

| Top hits | Sidewall hits | Bottom hits |
| :---: | :---: | :---: |
|  |  |  |
|  |  |  |
|  |  |  |
|  |  |  |



Figure 18: 2D trajectory plots at each trial beam energy of $4 \times 4$ array of $1 \mu \mathrm{~m}$ deep HAR hole. The trapezoids are the outline of the Boolean holes in $\mathrm{SiO}_{2}$ and the material underneath is Si .

Figure 18 helps determine the nature of the escaping electrons from holes at each energy. The case where electrons hitting middle of sidewall at $10-15 \mathrm{kV}$ seems to lead to more electrons escaping same hole, and with few exiting from hole bottom, that implies some contrast. Lower energies have fewer escaping, and higher energies have more escaping but many from other parts of sample which will be product of more scattering events and energy loss, so energy filtering of low loss BSE's (LLBSE) should be of large benefit in counting the real signal electrons, which makes sense from this collection of plots. As a last analysis, radial waveforms at hole bottom for each beam energy is shown in Figure 19.


Figure 19: Radial waveforms at each bream energy at hole bottom with $\mathrm{N}=1000$ electrons/pixel. Note the edge of the hole is at $\mathrm{x}=-85 \mathrm{~nm}$ as shown (relative scale to Cartesian coordinates in simulator), and the beam energies 10 kV through 25 kV seem to respond to the known hole edge such that there must be some sensitivity to hole bottom.

Physical imaging results of this case in the literature reports that these holes are best imaged experimentally at 10 kV with LLBSE electrons.[9] This simulation study thus confirmed the expected result.

## CONCLUSIONS

More complex features can now be modeled using AMAG SimuSEM, which uses JMONSEL's physics but through a powerful GUI, greatly improving utility, productivity, flexibility, visualization, accessibility, and achievable complexity of designed features with greatly increased speed. In this work, SimuSEM was applied to cases of industry interest with more complexity than in past. Intricate Intentional Defect Array designs demonstrated ability to predict response to large variety of SNR signatures in same test, with defect types previously impossible to encode or visualize. True defined rough photoresist line segments can be simulated more realistically than in past, with ability to explore where signal is scattered, to understand how the profile, roughness and foot interact to define apparent meandering line edge. Photoresist footing was also explored, and simulations showed foot $<3 \mathrm{~nm}$ very difficult to detect in photoresist.
HAR holes with $1 \mu \mathrm{~m}$ depth were simulated, and the trajectories and BSE signals showed bottom edge location most detectible in the $10-20 \mathrm{kV}$ range, consistent with reported experimental results. And those signals should be most likely improved with LLBSE filtering, as shown by the trajectory images.

SimuSEM demonstrated the ability to systematically define and evaluate SEM performance on very small details to allow careful DOE work to be done on such cases, which is important for model-based metrology/algorithm development and calibration, Hybrid metrology comparisons involving SEM, HV-SEM/Overlay exploration and reference metrology, SEM imaging condition optimization, limits/gaps analysis and feasibility studies, faux image
generation for AI training, calibration of analytical models, or to fundamental understanding of signal generation in tough cases such as roughness. Over the next year, we expect to add rigorous meshing solutions to allow user-defined roughness, new sample definition and image analysis and comparison features, charging capability, and more.

## ACKNOWLEDGEMENTS

AMAG Consulting, LLC thanks Dr. John S. Villarrubia of the National Institute of Standards and Technology (NIST) in Gaithersburg, Maryland, USA. Dr. Villarrubia is the creator of the JMONSEL SEM simulation software that is the physics core and basis for SimuSEM. Thanks also goes to Dr. David Klotzkin of SUNY Binghamton.

## REFERENCES

[1] Liddle, J. A., Hoskins, B. D., Vladár, A. E. and Villarrubia, J. S. "Research Update: Electron beam-based metrology after CMOS", APL Materials 6, 070701 (2018); https://doi.org/10.1063/1.5038249 .
[2] Villarrubia, J. S., et al., "Scanning electron microscope measurement of width and shape of 10 nm patterned lines using a JMONSEL-modeled library", Ultramicroscopy (2015), http://dx.doi.org/10.1016/j.ultramic.2015.01.004 .
[3] Villarrubia, J. S. , Ritchie, N. W. M., and Lowney, J. R. "Monte Carlo modeling of secondary electron imaging in three dimensions," Proc. SPIE 6518, 65180K (2007).
[4] J. R. Lowney, A. E. Vladár, and M. T. Postek, "High-accuracy critical-dimension metrology using a scanning electron microscope," Proc. SPIE 2725, pp. 515-526 (1996); J. R. Lowney, "Application of Monte Carlo simulations to critical dimension metrology in a scanning electron microscope," Scanning Microscopy 10, pp. 667-678 (1996).
[5] J. S. Villarrubia and Z. J. Ding, "Sensitivity of SEM width measurements to model assumptions," Proc. SPIE 7272 (2009).
[6] Villarrubia, J. S., and Ding, Z. J. "Sensitivity of SEM width measurements to model assumptions," J. Micro/Nanolith. MEMS MOEMS 8, 033003 (2009).
[7] J. S. Villarrubia, A.E.Vladár, B.Ming, R.J.Kline, D.F.Sunday, J.S.Chawla, and S.List, "Scanning electron microscope measurement of width and shape of 10 nm patterned lines using a JMONSEL-modeled library," Ultramicroscopy 154 (2015) 15. http://dx.doi.org/10.1016/j.ultramic.2015.01.004
[8] Benjamin Bunday. "Noise fidelity in SEM simulation". Proc. SPIE, Volume 11325, Metrology, Inspection, and Process Control for Microlithography XXXIV; 113250R (2020). https://doi.org/10.1117/12.2559631
[9] Benjamin Bunday, Abner Bello, Eric Solecky \& Alok Vaid, "7/5 nm logic manufacturing capabilities and requirements of metrology", Proc. SPIE 10585, Metrology, Inspection, and Process Control for Microlithography XXXII, 105850I (22 March 2018); doi: 10.1117/12.2296679
[10] Chris A. Mack and Benjamin D. Bunday. "CD-SEM algorithm optimization for line roughness metrology", Proc. SPIE 10585, Metrology, Inspection, and Process Control for Microlithography XXXII, 105850G (19 March 2018); doi: $10.1117 / 12.2297426$
[11] Maseeh Mukhtar, Benjamin Bunday, Kathy Quoi, Matt Malloy \& Brad Thiel. "Measuring multielectron beam imaging fidelity with a signal-to-noise ratio analysis", J. Micro/Nanolith. MEMS MOEMS 15(3) 034004 doi: 10.1117/1.JMM.15.3.034004, Published in: Journal of Micro/Nanolithography, MEMS, and MOEMS Volume 15, Issue 3 (23 August 2016).
[12] Benjamin Bunday, Maseeh Mukhtar, Kathryn Quoi, Bradley Thiel, \& Matt Malloy. "Simulating Massively Parallel Electron Beam Inspection for sub-20 nm Defects". Proceedings of SPIE Vol. 9424, 94240J (2015).
[13] Brad Thiel, Michael Lercel, Benjamin Bunday \& Matt Malloy, "Assessing the Viability of Multi-Electron Beam Wafer Inspection for sub-20 nm Defects", Proc. SPIE 9236, Scanning Microscopies 2014, 92360E (2014); doi:10.1117/12.2069302.
[14] Aron Cepler, Benjamin Bunday, Bradley Thiel \&John Villarrubia. "Scanning electron microscopy imaging of ultrahigh aspect ratio hole features". Metrology, Inspection, and Process Control for Microlithography XXVI. Proceedings of the SPIE, Volume 8324, pp. 83241N-83241N-14 (2012).
[15] Maseeh Mukhtar, Bradley Thiel \& Benjamin Bunday. "Backscattered electron simulations to evaluate sensitivity against electron dosage of buried semiconductor features", Proc. SPIE. 10585, Metrology, Inspection, and Process Control for Microlithography XXXII (2018).
[16] Thiel, B., Mukhtar, M., Quoi, K., Bunday, B., \& Malloy, M. (2016). Patterned Wafer Inspection with Multi-beam SEM Technology. Microscopy and Microanalysis, 22(S3), 586-587. doi:10.1017/S1431927616003780
[17] K. T. Arat, T. Klimpel, and C. W. Hagen "Model improvements to simulate charging in SEM", Proc. SPIE 10585, Metrology, Inspection, and Process Control for Microlithography XXXII, 1058518 (13 March 2018); https://doi.org/10.1117/12.2297478
[18] Benjamin Bunday et al. "Electron-beam induced photoresist shrinkage influence on 2D profiles", Proc. SPIE 7638, Metrology, Inspection, and Process Control for Microlithography XXIV, 76381L (1 April 2010); https://doi.org/10.1117/12.846991
[19] B. Bunday, C. Montgomery, W. Montgomery \& A. Cepler. "Photoresist shrinkage effects in 16 nm node EUV photoresist targets". Proc SPIE v8681, 86810J (2013).
[20] Benjamin Bunday, Aaron Cordes, Carsten Hartig, John Allgair, Alok Vaid, Eric Solecky, Narender Rana. "Timedependent electron-beam induced photoresist shrinkage effects". J. Micro/Nanolith. MEMS MOEMS. 11(2), 023007 (Jun 05, 2012). doi:10.1117/1.JMM.11.2.023007
[21] Benjamin Bunday, Cecilia Montgomery, Warren Montgomery, and Aaron Cordes. "Static and dynamic photoresist shrinkage effects in EUV photoresists". Metrology, Inspection, and Process Control for Microlithography XXVI. Proceedings of the SPIE, Volume 8324, pp. 83241E-83241E-16 (2012).
[22] Benjamin Bunday, Aaron Cordes, Andy Self, Lorena Ferry, and Alex Danilevsky. "Experimental validation of 2-D profile photoresist shrinkage model". Metrology, Inspection, and Process Control for Microlithography XXV. J. Proceedings of the SPIE, Volume 7971, 79710W (2011).
[23] Bunday, B., Cordes, A., Allgair, J., Tileli, V., Avitan, Y., Peltinov, R., Bar-zvi, M., Adan, O., Cottrell, E., and Hand, S. "Phenomenology of electron-beam-induced photoresist shrinkage trends". Proc. SPIE, Vol. 7272, 72721B-1-15 (2009). Winner of SPIE Metrology 2009 Diana Nyyssonen Award for Best Paper of Conference.
[24] See details on Blender at website: https://www.blender.org/.
[25] Bunday, B., McCormack, D., Bishop, M., Villarrubia, J., Vladar, A., Dixson, R., Vorburger, T., Orji, N, and Allgair, J. "Determination of Optimal Parameters for CD-SEM Measurement of Line Edge Roughness". Proceedings of the SPIE: Metrology, Inspection, and Process Control for Microlithography XVIII (2004), 515-533.
[26] Villarrubia, J. and Bunday, B. "Unbiased Estimation of Linewidth Roughness". Procedings of SPIE 2005, v5752, pp 480-488. Winner of SPIE Metrology 2005 Diana Nyyssonen Award for Best Paper of Conference.

