Scanning electron microscope measurement of width and shape of 10 nm patterned lines using a JMONSEL-modeled library

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The width and shape of 10 nm to 12 nm wide lithographically patterned SiO₂ lines were measured in the scanning electron microscope by fitting the measured intensity vs. position to a physics-based model in which the lines' widths and shapes are parameters. The approximately 32 nm pitch sample was patterned at Intel using a state-of-the-art pitch quartering process. Their narrow widths and asymmetrical shapes are representative of near-future generation transistor gates. These pose a challenge: the narrowness because electrons landing near one edge may scatter out of the other, so that the intensity profile at each edge becomes width-dependent, and the asymmetry because the shape requires more parameters to describe and measure. Modeling was performed by JMONSEL (Java Monte Carlo Simulation of Secondary Electrons), which produces a predicted yield vs. position for a given sample shape and composition. The simulator produces a library of predicted profiles for varying sample geometry. Shape parameter values are adjusted until interpolation of the library with those values best matches the measured image. Profiles thereby determined agreed with those determined by transmission electron microscopy and critical dimension small-angle x-ray scattering to better than 1 nm.

Keywords: Critical dimension (CD); critical dimension small angle x-ray scattering (CD-SAXS); dimensional metrology; model-based metrology; scanning electron microscopy (SEM); transmission electron microscopy (TEM); simulation.

1. Introduction

Some of the most demanding requirements for accuracy and repeatability of dimensional measurements made with the scanning electron microscope (SEM) come from the semiconductor electronics industry. The International Technology Roadmap for Semiconductors[1] says sub 20 nm physical gate lengths should be typical in 2016. Manufacturing tolerances permit only 1.6 nm of size variation in this critical dimension (CD). This in turn requires no more than 0.29 nm of uncertainty in the CD metrology tool's measurements of dense lines. (These variations are 3 standard deviations.)

By 2020, 12.5 nm gates will require measurements with 0.21 nm uncertainty. Increased use of pitch-splitting techniques and fabrication of FinFETs (a kind of multi-gate field effect transistor, in production since 2012) produce similar CD tolerances but also introduce new critical process parameters, such as sidewall angle and height.

Uncertainty in the width of a line is determined by the uncertainty in the locations of its edges. On the Si wafer, a FinFET's fin is topographically a raised line. In the SEM image, the edges of this line are brighter than their surroundings because the secondary electrons (SE) generated by the beam reach the detector more easily when there are two channels of escape (top and side of the line, when the beam is near the edge) than when there is one (top only, when the beam is far from the edge). The region of increased brightness is some nanometers in extent. The location of the actual edge within this region is not known *a priori*, and it may, moreover, depend upon secondary (and variable) sample characteristics, such as the shape of the line edge, its angle,

[†]. Certain commercial equipment, instruments, or materials are identified in this paper in order to specify the experimental procedure adequately. Such identification is not intended to imply recommendation or endorsement by the National Institute of Standards and Technology, nor is it intended to imply that the materials or equipment identified are necessarily the best available for the purpose.

the proximity of neighboring lines, etc. These are all, therefore, substantial contributors to measurement uncertainty.

Our approach to the measurement problem has three parts: (1) a Monte Carlo simulator with physics models of the electron beam/sample interaction that predicts the intensity, $I(x, y; \mathbf{p})$ as a function of position (x, y) that should be measured for given vector, $\mathbf{p}$, the components of which are parameters (beam size, linewidth, sidewall angle, ...) that describe the instrument and sample geometry, (2) a nonlinear least-squares fitting algorithm to determine the value of $\mathbf{p}$ that produces the best match between the simulated and measured images, and (3) a fast approximation of the model by interpolation of a library of discretely sampled model results. Earlier, this approach was demonstrated on silicon and photoresist lines with widths greater than 50 nm.[2-5] In those studies, the best matching trapezoidal lines agreed with subsequent cross-sectional measurements to within the several nanometer measurement uncertainty, uncertainty dominated by sample roughness or resist shrinkage. This measurement method creates a linkage between a technologically important measurement and often uncertain fundamental physics (e.g., SE generation by slow primary electrons).

There are important differences between the earlier studies and the present work. The previous work used an earlier simulator called MONSEL.[6,7] It employed different models for elastic scattering, SE generation, and boundary crossing and had a more restricted repertoire of sample shapes than does the present study's JMONSEL (Java Monte Carlo simulator for Secondary Electrons). An overview of JMONSEL is given in Sec. 2. The physics it employs is described in Sec. 3. These simulation and modeling capabilities were applied to measurements of a sample fabricated at Intel using a pitch quartering technique that resulted in approximately 10 nm (top width) lines at 32 nm spacing. The sample and experimental procedures are described in Sec. 4. These lines are significantly narrower and more complicated in shape than the earlier ones. The earlier linewidths in excess of 50 nm meant the intensity at one line edge was independent of the distance to the opposite edge, and the independent edges approximation[2] was valid. At 10 nm, this is no longer true, and it is necessary to model combinations of edge shapes for both edges of the line for several different widths. Simulations and fits will be described in Sec. 5. Results will be given in Sec. 6 and compared to independent determinations of pitch, width, and shape by transmission electron microscopy (TEM) cross section and critical dimension small angle x-ray scattering (CD-SAXS).[8]

2. The JMONSEL simulator

2.1 Overview

JMONSEL is a Java package that extends Nicholas Ritchie's Electron Probe Quantification (EPQ) library.[9] The library as a whole contains a number of packages with utilities for describing materials and their properties relevant

FIG. 1. Schematic of some possible events that terminate a trajectory leg.

for interactions with electrons. One notable package, NIST-Monte, contains utilities for performing Monte Carlo simulations of electron trajectories through 3D samples. The EPQ library was originally written to support x-ray microanalysis. Its capabilities include simulation of x-ray generation, transmission, and detection, along with the resulting x-ray spectra. Electrons with energies too low to generate x-rays were either dropped or treated approximately, since they are of little interest for x-ray microanalysis. Low-energy phenomena are, however, important for SEM images, particularly SE images. JMONSEL adds capabilities for treating phenomena relevant for this kind of imaging.

Simulations are performed by executing programs written in Jython, a Java version of the Python scripting language. A typical script accesses NISTMonte and JMONSEL utilities to define the sample geometry and materials, choose from among available scattering models for each material, define electron gun properties, and initialize detectors. Then a specified number of beam electrons are simulated, after which detectors are polled to determine the resulting signal (usually yield). The above steps are typically run in a loop, in which the signal is computed as a function of varying inputs. Depending upon which inputs are varied, the result may be yield vs. position (an image), yield vs. beam energy, yield vs. angle of incidence, yield vs. position and sample shape (e.g., to make a library), etc.

During simulation, the electron motion is divided into steps or trajectory legs. The electron's position, energy, and direction of motion at the beginning of the first leg are determined by the electron gun. In each subsequent leg, they are equal to the values on completion of the previous leg. Possible events that end each leg are shown in Fig. 1. The primary electron may scatter before it reaches a material boundary, in which case it may or may not generate an SE, depending on the type of scattering event. Alternatively, if it reaches the boundary, it either transmits or reflects.

The leg begins with a move along the electron's initial direction of motion. The length of the move is the smaller of (1) the distance to the next boundary crossing or (2) the electron's scattering free path. The scattering free path, λ , is

$$\lambda = -\lambda_{\text{mfp}} \ln(R) \quad (1)$$

where R is a random number uniform between 0 and 1 and λ_{mfp} is the mean free path, given by

$$\lambda_{\text{mfp}}^{-1} = \sum_i \lambda_i^{-1}. \quad (2)$$

In Eq. (2), λ_i is the mean free path of the i^{th} scattering mechanism and the sum is over all scattering mechanisms that have been assigned to the material in which the electron resides. The random number and logarithm in Eq. (1) cause λ to be Poisson-distributed with mean value λ_{mfp} . If the transport model in the electron's region includes a CSDA component, the electron's energy is decremented. (CSDA, or continuous slowing-down approximation, is one way of modeling energy loss that is sometimes used. See Sec. 3.7.) If the distance to the nearest boundary is less than the scattering free path, the electron's energy and direction of motion at the end of the leg are determined by the boundary crossing model (Sec. 3.6). Otherwise, the scattering mechanism that terminated the leg is deemed to be one chosen randomly from the list with probabilities weighted by their respective inverse mean free path values. The chosen scattering mechanism determines the electron's final energy, direction, and whether or not an SE is generated. The last step in the trajectory leg is to drop the electron from further simulation if the drop condition has been met. Typically this is based on the electron's final energy or whether a scattering event (e.g., a trap) has specified that the trajectory is to end.

2.2 Geometrical representations

The simulation space is divided into regions, each uniform in composition. The shape of each region is represented internally by constructive solid geometry (CSG). In CSG, 3D primitives (e.g., spheres, cylinders, polyhedra; See Fig. 2a) are combined using basic set operations (union, intersection, difference,...) to make more complex shapes. The representation is hierarchical. The root of the hierarchy is a spherical chamber region. New regions (e.g., parts of the sample or detectors) are added as subregions of the chamber. These new regions may themselves have subregions, nesting in this way ordinarily to any depth. Shapes may be transformed by any affine transformation (translation, rotation, scaling, skewing,...) before or after combination.

Shapes may also be represented by height maps. A basic height map is a 2D array of heights on a regularly spaced x, y grid. It represents a sampling of a single-valued function at regular intervals. A conventional atomic force microscope image, for example, is a height map. It is a convenient representation for complicated or rough surfaces. The height map is internally converted into a CSG representation, so it may be subsequently transformed and combined with other shapes, including other height maps (Fig. 2b).

Finally, there is provision for tetrahedrally meshed regions (Fig. 2c). The tetrahedral mesh is imported from a file in the format used by Gmsh,[10] a freely available (GNU General Public License) meshing software. The tetrahedra

FIG. 2. Geometrical representations: (a) Constructive solid geometry uses shape primitives (left) and set operations to produce combined shapes (right). (b) Height maps with “inside” defined below (left) or above (middle) the pictured surface and their intersection (right). (c) Tetrahedral meshed sample and surrounding vacuum.

are internally converted to modified CSG shapes. The modifications add some capabilities (assignment of electrical potentials to nodes and methods that solve for electric fields or potentials in the interior) and remove others (ability to have subregions) to make their use with finite element analysis software possible. JMONSEL requires the use of meshed regions if the effects of charging are to be modeled.

2.3 Materials

A region is specified by the shape of its boundary (Sec. 2.2) and the properties of the material it contains. The specification, in the form of a “MaterialScatterModel,” includes the following:

1. The material's elemental composition, stoichiometry, density, and basic electronic properties: work function, Fermi energy, band gap, etc.
2. Scattering properties of electrons in the material. These include the free path as a function of energy and a method to compute the outcome of a scattering event, including the new direction and energy of the primary electron and the energy and direction of an SE if the scattering event generates one. Usually this scattering is determined from a list of operative mechanisms from Sec. 3.2 through Sec. 3.5. For example, we might have an elastic (electron-nuclear) scattering mechanism from Sec. 3.2, a SE generation mechanism from Sec. 3.3, and possibly phonon scattering or electron trapping mecha-

nisms if these are significant for the material in that region.

3. A method to handle boundary crossings for electrons that leave this material. This method determines the electron's new energy and direction of motion, including whether it transmits or reflects at the boundary.
4. A continuous slowing down model (CSDA) for this material. This specifies the amount of energy lost by an electron as a function of its initial energy and distance traveled in the material. The continuous loss amount may be set to zero, for example if all energy losses are already included in discrete inelastic scattering models.
5. A minimum electron energy, below which the electron is dropped from the simulation.

2.4 Detectors

The simulator generates events at significant times, e.g., the beginning of the first of a set of multiple trajectories, at the beginning and end of each individual trajectory in the set, at each scattering event, when a SE is generated or its trajectory ends, when an electron crosses a region boundary or strikes the chamber wall. Detectors register to be notified of these events and take some action, such as recording statistics, when so notified.

One such detector generates trajectory plots for all or a limited number of trajectories. Another generates a log file with detailed information about trajectories: the coordinates and energy at the endpoints of each leg, the kind of event (boundary crossing, scattering, etc.) that terminated the leg, etc. The log file can be mined for information in subsequent analysis. Yet another detector records statistics about electrons that hit the chamber wall: histograms, counts of electrons vs. energy and angle for each of forward- and back-scattered electrons. The ratio of total counts in the histogram to number of incident electrons is the total yield. Subsets of the histogram are also often important. So, for example, the ratio of counts in bins less than 50 eV to incident electrons is conventionally the SE yield, δ , while that for bins greater than 50 eV is the backscattered electron (BSE) yield, η . A "RegionDetector" keeps similar histograms for electrons that enter a specified list of regions in the simulation space. These regions could, for example, be placed at a realistic location in order to monitor an actual detector placement. Alternatively, such a detector could be placed at a position of interest inside the sample, where no physical detector is possible, as a kind of simulation monitor. Zero or more instances of each kind of detector may be independently configured.

3. Models

This section describes the physics in the most commonly used of JMONSEL's models. Not all of the models listed here are used in any particular simulation. Some of these, for example, are different models for the same phenomenon.

Which of these to use is specified by the simulation script as part of the initialization of the MaterialScatterModel.

3.1 Electron gun

The electron gun simulator takes as inputs a best focus coordinate, a beam width (σ), a direction vector, and an angular aperture, α . It generates electrons that converge to a focal plane, where arriving electrons are normally distributed with standard deviation σ in each of the x and y directions. The mean direction of the electrons is given by a supplied direction vector (vertical by default), but individual electrons deviate from the mean direction by random azimuthal and polar angles ϕ and θ . The azimuthal angle is uniformly distributed from 0 to 2π , while $\cos\theta$ is uniform between 1 and $\cos\alpha$. Thus, the beam is shaped like an hourglass, with electrons converging prior to the point of best focus and diverging after, the cone half angle equal to the supplied angular aperture, all directions within the cone equally likely, and a normally distributed density of electrons within the spot at best focus.

3.2 Elastic scattering

Scattering of electrons from atomic nuclei is responsible for almost all large-angle scattering, particularly when the primary electron has energy large compared to typical SE energies (a few tens of electron volts), and for this reason it is largely responsible for the interaction volume (the region into which electrons spread within the sample) not being confined near the beam axis. Because even lightweight nuclei are thousands of times more massive than electrons, electron energy loss is negligible in these collisions.

JMONSEL has a number of scattering algorithms available for computing free paths and scattering angles in these events. One is based on the screened Rutherford differential cross section. Its simple analytical form has made it popular in earlier simulators. However, the Mott cross sections[11] are more accurate, particularly for low energies or heavy elements. For this reason JMONSEL has three other algorithms representing approximations of the solution of Mott's scattering equations. One of these, designated NISTMott, uses an interpolation of tabulated Mott scattering cross sections in NIST Standard Reference Database 64.[12] These tables were computed by the partial wave expansion method with the Dirac-Hartree-Fock potential.[13] The tables cover primary electron energies in the range 50 eV to 20 keV. Another one, designated CzyzewskiMott, uses tables from 20 eV to 30 keV produced by Czyzewski et al.[14] A third, designated BrowningMott, uses an empirical analytical fit to the Mott cross sections developed by Browning.[15-17] We commonly use a hybrid of three of these: NISTMott for $50 \text{ eV} \leq E \leq 20 \text{ keV}$ where the tables are valid, screened Rutherford for $E > 20 \text{ keV}$, and extrapolation below 50 eV according to Browning's formula.

3.3 Secondary electron generation

3.3.1 Dielectric function theory model

JMONSEL has a choice of two SE generation modules. The first, designated `TabulatedInelasticSM`, is not, properly speaking, a model. Rather, it determines the inelastic free path and the result of a scattering event with the aid of several tables that it imports. The model is thereby implicitly contained in the tables. Four tables are required. The first tabulates $\lambda_{\text{mfp}}^{-1}$ vs. E (inverse inelastic mean free path vs. primary electron energy). It is used to determine a random Poisson-distributed free path via Eq. (1). The second tabulates the primary electron's energy loss, ΔE , vs. E and R_1 . (In this paper R will always designate a random number uniformly distributed between 0 and 1. Varying subscripts indicate independent random numbers.) The third tabulates the angular deflection, θ , of the primary electron as a function of E , ΔE , and R_2 (though, since the allowed range of ΔE varies with E , a reduced energy scale is used for ΔE , in which 0 corresponds to the minimum and 1 to the maximum allowed value). The azimuthal angular deflection is uniform from 0 to 2π . That is, this module assumes materials are isotropic. This module assumes all of the ΔE lost by the primary electron is transferred to an SE. This electron already has some energy E_{SE0} relative to the bottom of its band. Thus, its final energy relative to the bottom of the conduction band is

$$E_{\text{SE}} = E_{\text{SE0}} + \Delta E + E_s - E_c \quad (3)$$

where $E_s - E_c$ is the energy difference between the “scattering band” (the band in which the SE originally resides) and the conduction band. Since electrons in the scattering band do not all have the same energy, the value of E_{SE0} in a given collision follows a random distribution supplied by the fourth table, which gives E_{SE0} vs. ΔE and R_3 .

All of the scattering tables presently available in JMONSEL are based upon dielectric-function theory (DFT), which gives the differential inverse inelastic mean free path by[18]

$$\frac{d^2 \lambda_{\text{in}}^{-1}}{d(\hbar\omega)dq} = \frac{1}{\pi a_0 E} \text{Im} \left[-\frac{1}{\varepsilon(q, \omega)} \right] \frac{1}{q} \quad (4)$$

with $\hbar\omega = \Delta E$ the energy loss and q the momentum change of the primary electron, a_0 the Bohr radius (≈ 0.053 nm), E the energy of the incident electron, and $\varepsilon(q, \omega)$ the complex dielectric function including finite momentum transfer. Conservation of energy and momentum establish a relationship between q and the scattering angle, θ .

$$\frac{(\hbar q)^2}{2m} = 2E - \Delta E - 2\sqrt{E(E - \Delta E)} \cos \theta. \quad (5)$$

This relation allows a change of variable from q to θ in Eq. (4). Consequently, for given E and ΔE , the right hand side after normalization prescribes the third of `TabulatedInelasticSM`'s required tables. Integration over all scattering angles (or equivalently all allowed q values) pro-

duces the second of the required tables: the probability of ΔE given E . Finally, integration over all allowed ΔE gives λ_{in}^{-1} vs. E , which is the first table.

To compute the tables, Eq. (4) is evaluated using Penn's method[19] of expressing $\text{Im}[-1/\varepsilon(q, \omega)]$ in terms of an integral expansion using Lindhard free electron dielectric functions[20] with the expansion coefficients given in terms of the measured optical ($q = 0$) energy loss function (ELF), $\text{Im}[-1/\varepsilon(0, \omega)]$. Our method uses Penn's empirical plasmon dispersion relation[19] and follows closely that of Ding and Shimizu,[21] which can be consulted for details. Kieft and Bosch[22] have recently implemented a similar DFT-based model, but with a simpler dispersion relation.

The energy and momentum lost by the primary electron are assumed transferred to an SE. This electron's final energy and momentum depend also upon their initial values, which are unfortunately not specified by the DFT theory, so additional assumptions are required. Inelastic scattering events are separated into electron-electron and electron-plasmon types depending upon the momentum transfer, q , as described by Jensen and Walker[23] and Mao et al.[24].

An event is deemed to be electron-electron scattering if $(\sqrt{E_F + \Delta E} - \sqrt{E_F})^2 \leq (\hbar q)^2 / (2m) \leq (\sqrt{E_F + \Delta E} + \sqrt{E_F})^2$, with E_F the Fermi energy. In this case, conservation of energy and momentum require $(\hbar k_0)^2 = 2mE_{\text{SE0}}$, $(\hbar k_f)^2 = 2m(E_{\text{SE0}} + \Delta E)$, and $\mathbf{k}_f = \mathbf{k}_0 + \mathbf{q}$, which imply $\mathbf{k}_0 \cdot \mathbf{q} = m\Delta E / \hbar^2 - q^2 / 2$. For fixed $\mathbf{q}$ and ΔE , this is the equation of a plane. Thus the SE's initial momentum must lie within a planar slice through the Fermi sphere. We choose $\mathbf{k}_0$ at random with equal weight from among the allowed possibilities (in the required plane, with initial energy less than E_F and final energy greater than E_F). This is the same method as Mao et al.[24] Once $\mathbf{k}_0$ is chosen, the SE's final energy and direction are completely determined.

If the condition for electron-electron scattering is not met, the event is deemed to be a plasmon excitation. Then E_{SE0} is determined by `TabulatedInelasticSM`'s fourth input table, presently constructed to assign E_{SE0} randomly from the interval $[E_F - \Delta E, E_F]$ with probability proportional to the joint density of states, $\sqrt{E_{\text{SE0}}(E_{\text{SE0}} - \Delta E)}$, as described by Ding et al.[25] An isotropic random direction is assigned.

3.3.2 Fitted inelastic scattering model

One of the oldest methods for estimating SE yields has its roots in ideas of Salow[26], expanded upon by others.[27-31] In this model the inverse inelastic mean free path is

$$\lambda_{\text{in}}^{-1} = -\frac{1}{\varepsilon} \frac{dE}{ds}. \quad (6)$$

$dE/(ds)$ is the rate of energy change per unit distance traveled (stopping power), and ε is a characteristic energy required to produce an SE. Previous implementations of this model were for planar samples, where the generated electron is at a well-defined depth, z , below the surface. The probability that this electron would escape was modeled with an

exponential form, proportional to $e^{-z/d}$, with d a characteristic escape depth, and the yield was computed immediately, with no need to follow the trajectory of the generated electron. Even if the stopping power for the material is known, this model has at least two unknown parameters, ε and d , the values of which are typically assigned to produce the best fit between measured and modeled yield vs. energy. Lin and Joy[31] have tabulated values for a number of materials.

In JMONSEL the implementation of this model must differ because the sample may be arbitrarily complex. It is for this reason difficult to efficiently determine the distance to the nearest escape surface, which moreover need not be a plane. For this reason JMONSEL's FittedInelasticSM instantiates an electron with energy ε and isotropically random direction at each scattering event of this type. That electron is then tracked along with subsequent scattering events, energy loss, etc. In this way the Monte Carlo averages over a sample of possible escape paths to determine the yield. Tracking electrons with energy below 50 eV requires the stopping power model to be valid at those energies. The FittedInelasticSM model is usually used when good ELF data are unavailable, in which case the low-energy stopping power has significant uncertainty. Consequently, the stopping power itself often has a free parameter that is also adjusted, along with ε , to fit the measured yield curve. Thus, this implementation, like the earlier ones, has two fitted parameters.

This is a cruder model than the DFT one in Sec. 3.3.1, inasmuch as it has more fitting parameters, and SE are generated with a single, average, energy instead of a more realistic distribution of energies. Its advantage is that it does not require the ELF function to be known. There are no existing measurements of ELF's for many materials imaged in semiconductor electronics and other applications. Because the prerequisites are less demanding, the FittedInelasticSM can often be used in such cases.

3.4 Phonon scattering

In metals or in insulators at primary electron energies more than several times the band gap, inelastic scattering is dominated by electron-electron interactions. However, when the ordinarily dominant mode goes to zero, as for example for primary electron energies less than an insulator's nonzero band gap, the electron range becomes unrealistically approximated by infinity unless the most important of the remaining inelastic channels is modeled. JMONSEL includes a longitudinal optical phonon scattering model based on that of Llacer and Garwin[32]. Ganachaud and Mokrani[33] and Dapor et al.[34] also used this model, which has its roots in Fröhlich's[35,36] perturbation theory. In this model the inverse inelastic mean free path for creating a phonon is

$$\lambda_{\text{ph}}^{-1} = \frac{n}{2} \left(1 + \frac{1}{e^{\frac{E_{\text{ph}}}{kT}} - 1} \right) \left(\frac{1}{\varepsilon_{\infty}} - \frac{1}{\varepsilon_0} \right) \frac{x}{a_0} \ln \left(\frac{1 + \sqrt{1-x}}{1 - \sqrt{1-x}} \right) \quad (7)$$

with E_{ph} the energy of the phonon, n the number of phonon modes at this energy, kT the Boltzmann factor, ε_0 and ε_{∞} the static and optical dielectric constants, a_0 the Bohr radius, and $x = E_{\text{ph}}/E$ the ratio of phonon to electron energy. The opposite process, in which a phonon is annihilated with the electron gaining its energy, is much less probable at temperatures encountered in the SEM and is neglected.

The scattering angle is given by

$$\cos \theta = \frac{2-x}{2\sqrt{1-x}} (1 - B^{R_4}) + B^{R_4} \quad (8)$$

with R_4 uniformly distributed between 0 and 1 and

$$B = \frac{2-x+2\sqrt{1-x}}{2-x-\sqrt{1-x}}. \quad (9)$$

The azimuthal angle is uniformly distributed between 0 and 2π . Whenever $x < 0.1$ (almost always the case) JMONSEL branches to faster expressions that retain only low order terms in expansions of Eq. (7) and Eq. (8).

3.5 Electron trapping

Ganachaud and Mokrani modeled the probability per unit path length of an electron becoming trapped by

$$\lambda_{\text{trap}}^{-1}(E) = S_{\text{trap}} e^{-\gamma_{\text{trap}} E}. \quad (10)$$

JMONSEL also has an implementation of this model. S_{trap} and γ_{trap} are user-supplied input parameters. If the electron's trajectory leg ends by trapping, the trajectory terminates.

3.6 Material boundary crossing

The potential energy change at a material boundary causes refraction or reflection and a kinetic energy change. We adopt an exponential s-curve for the form of the potential energy: $U(x) = \Delta U / [1 + \exp(-2x/w)]$, with x the perpendicular distance to the boundary. This form provides one parameter (ΔU , positive if the potential energy increases across the barrier) for the barrier height, and one (w) for the width. Schroedinger's equation can be solved analytically for the transmission probability. The solution for an electron incident at angle ϑ is[37]

$$T(E, \vartheta) = \begin{cases} 1 - \left(\frac{\sinh \left[\frac{1}{2} \pi w (k_1 - k_2) \right]}{\sinh \left[\frac{1}{2} \pi w (k_1 + k_2) \right]} \right)^2 & E \cos^2 \vartheta > \Delta U \\ 0 & \text{otherwise} \end{cases} \quad (11)$$

with $\hbar k_1 = \sqrt{2mE \cos^2 \vartheta}$, $\hbar k_2 = \sqrt{2mE \cos^2 \vartheta - \Delta U}$, m the electron's mass and E its energy. If w is small compared to the electron wavelength this formula reduces to the abrupt quantum mechanical barrier used by others.[21,34] In the opposite limit, it becomes a classical barrier.

If the electron does not transmit, it reflects specularly. If it transmits it refracts. Its perpendicular component of momen-

tum becomes $p_{\perp}^2 = p_{0\perp}^2 - 2m\Delta U$ with $p_{0\perp}$ the initial perpendicular component. The momentum parallel to the barrier is unchanged.

3.7 Stopping power

The stopping power, $-dE/ds$, is the electron's average rate of energy loss per unit distance traveled. It is a function of the material and the electron's energy. Some models, e.g., the DFT model in Sec. 3.3.1, do not require a stopping power model as input. Rather, the stopping power is an output. Such models are attractive when available because they conserve energy in detail, i.e., in each collision, and the energy loss that accompanies traversal of a given distance has a realistic distribution over a range of values. However, as mentioned above, the required material data are not always available to implement such a model. A less detailed treatment is also sometimes preferable. For example, it is possible to speed simulations by dispensing with SE generation models altogether for interior parts of the sample from which SE cannot escape, provided the primary electron's energy loss is otherwise taken into account.

Models like the fitted inelastic scattering model of Sec. 3.3.2 take a stopping power model as input. This is possible because there are simple expressions for stopping power as a function of energy and material properties, for example the well-known Bethe stopping power[38,39]. Bethe's form breaks down at low energies relevant for SEM imaging. Joy and Luo [40] and Rao-Sahib and Wittry [41] used different methods to extend Bethe's formula to lower energies. JMONSEL has an implementation of the Joy and Luo result, which is

$$\frac{dE}{ds} = -\alpha \frac{\rho}{E} \sum_i \frac{c_i Z_i}{A_i} \ln \left[1.166 \left(\frac{E}{J_i} + k_i \right) \right] \quad (12)$$

with ρ the material density, i an index of the material's elemental constituents, c_i , Z_i , A_i , and J_i respectively the weight fraction, atomic number, molar mass, and average ionization energy of the i^{th} constituent, α a constant (approximately $2.02 \times 10^{-31} \text{ J}^2 \text{ m}^2$ in SI units) and k_i a dimensionless constant, approximately 0.85 but material dependent, tabulated for several elements by Joy and Luo. This form extends the range of validity of the stopping power expression, but even this form was not claimed to be valid for $E < 50 \text{ eV}$.

For electrons with energies not too far above the Fermi level, Nieminen[42] found the stopping power to be proportional to $E^{5/2}$. An alternative JMONSEL implementation, designated JoyLuoNieminenCSD, uses Eq. (12) for $E > E_b$ and a Nieminen-like stopping power ($-\gamma E^{5/2}$) for $E \leq E_b$, with γ chosen to match them at E_b . Then E_b becomes a parameter that can be adjusted, for example to maximize agreement with a measured stopping power or yield curve. A comparison of several models is shown for Cu in Fig. 3.

FIG. 3. Low-energy comparison of stopping power models and measurements for Cu. The horizontal axis is kinetic energy referenced to the bottom of the conduction band. Measured data are from Hovington et al.,[43] Luo et al.,[44] and Al-Ahmad and Watt,[45] tabulated by Joy [46].

3.8 Charging

For semiconductor electronics metrology it is frequently necessary to make measurements on samples with insulating regions, for example the thick oxides that separate the metalized layers that form the circuit wiring, the contact holes through these layers, or insulating defect particles. This kind of simulation is performed in one or more meshed regions. Presently, the mesh is tetrahedral and produced by Gmsh[10] with variable element size: small where needed for accuracy (e.g., close to charged volumes) and larger elsewhere.

The i^{th} tetrahedral mesh element has an associated counter, n_i , that keeps track of the number of elementary charges trapped in that element. The counter is decremented whenever an electron's trajectory ends inside the element. It is incremented whenever an SE is generated inside the element. Thus the net charge in the element is always $n_i e$. Every N beam electrons, the scattering simulation pauses to allow the electrostatic potentials at the mesh nodes and the corresponding electric fields to be determined by finite element analysis (FEA). JMONSEL presently uses GetDP[47], a publicly available code, for this calculation. The FEA calculation permits three kinds of boundary conditions on volumes or surfaces of the mesh: Dirichlet (fixed potential), Neumann (fixed field), or floating (all nodes of a closed surface have the same potential, but the value of the potential depends on solution of the FEA taking into account the charge inside the volume). This is repeated every N electrons until the simulation finishes. The most recent solution of the fields is used to appropriately modify electron trajectories during the scattering portion of the simulation. N is a user-settable parameter. Larger values of N are associated with greater speed but lower accuracy. The chosen value represents a compromise.

FIG. 4. Repeated spacer deposition and etching results in 4 lines and spaces within each nominally 128 nm unit cell. The resulting lines stand on a layered substrate. Within each unit cell, lines and spaces are expected to follow an A-B-C-B pattern.

4. Experimental

4.1 Sample

To test the above model and library-based measurement plan, measurements were performed on a sample cleaved from a 300 mm wafer fabricated at Intel. The sample had both intentional (a small-variation focus-exposure matrix, or FEM) and unintentional (random natural process) dimensional variation.[48] The measured site was well inside ($>500\ \mu\text{m}$ from the nearest edge) of a 1 mm by 8 mm densely patterned area.

The sample processing, features, and dimensions were similar to those used for 34 nm metal pitch interconnect structures.[49,50] A spacer-based pitch quartering scheme (Fig. 4) places 4 lines and spaces into a unit cell that repeats at nominally 128 nm pitch. The lines are silicon dioxide. They reside on a layered substrate, first 30 nm of silicon nitride, then 25 nm of titanium nitride, then 100 nm of silicon dioxide, and finally the silicon wafer.

4.2 Measurements

4.2.1 Model-based library scanning electron microscopy (MBL-SEM)

The SEM was an FEI Helios NanoLab Dual-Beam instrument. Imaging conditions were: 4 mm working distance, 15 keV electron landing energy, 86 pA beam current, 100 ns pixel dwell time, 508 nm horizontal field of view, 512 pixels by 442 pixels in the horizontal and vertical directions respectively. Approximately 300 individual fast image frames were the inputs to generate the final images used in the model-based evaluation and three-dimensional reconstruction. The final images were generated by the NIST ACCORD software, which is a C library for composition of SEM or scanning helium-ion microscope images with correction of drift.[51] To compensate for drift and vibration, frames are

FIG. 5. Top-view secondary electron image of the sample after correlation shift and average. The field of view is approximately $508\ \text{nm} \times 418\ \text{nm}$.

shifted prior to averaging. The shift is chosen to maximize correlation using a two-dimensional Fourier transform-based method. The resulting image is compensated for a significant portion of these distortions, thereby eliminating much of the blur that otherwise results from averaging unshifted images. Because of drift and vibration, the individual fast image frames cover a somewhat larger area than the final image, which in size is equal to the individual images. The areas close to the edges have more noise (because some of the pixels fell outside the final image's area), so only the lines at the center portions of the final images were used in the model-based evaluation. A typical image is shown in Fig. 5. Edge assignments and the rectangular focus area will be discussed in Sec. 6. Four images like this were analyzed. They were sampled from different areas of the same pattern to assess site to site variation.

4.2.2 Transmission electron microscopy (TEM)

Cross-section bright field imaging of 24 nm to 34 nm pitch silicon dioxide features was carried out on an FEI Tecnai TEM at 200 keV. The cross-section sample lamella was capped using hand dispensed *BIC Mark it* ink. The ink filled features of 10 nm-12 nm and is lower stress than conventional cap materials like Pt and TEOS. The ink cap favors in sample imaging with negligible dimension and profile distortion from stress and high energy secondary electron interaction during focused ion beam sample preparation. The TEM sample preparation and imaging technique are discussed in detail in Ref 52. TEM cross-sections were imaged from a number of sites at different focus and exposure. The one taken from a site with similar focus/exposure to the site

FIG. 6. CD-SAXS geometrical shape model.

measured by SEM is analyzed in Sec. 6.2.

4.2.3 Critical dimension small angle x-ray scattering (CD-SAXS)

CD-SAXS measurements were performed at the 5-ID-D beamline at the Advanced Photon Source (APS). The beam energy was 17 keV, and the spot size was approximately 100 μm . A CCD detector was used to measure the scattering pattern and was calibrated from the scattering pattern of a grating sample of known pitch. Samples were mounted on a rotational stage. The center of rotation of the stage was aligned with the incident beam. The sample incidence angle was rotated from -60° to $+40^\circ$ from normal incidence in increments of 1° . The sample acquisition time was 10 s per angle. Scattering patterns at individual angles were transformed to a 2D reciprocal space map by projecting the scattering angle into its x and z components.

The periodic nanostructure shape was determined by using an inverse method where the experimental diffraction pattern was compared to the scattering pattern simulated from a trial shape solution. The trial shape was iterated until a match to the experimental data was obtained. The simulated scattering intensity of the trial shape was calculated and convolved with a one dimensional lattice:

$$I_0(q) \propto \int_A \rho(r) * \sum_n \delta(x - nP) e^{-iq \cdot r} dr \quad (13)$$

with ρ the electron density, δ the Dirac delta function, x the position on the 1D lattice, n the unit cell index (the sum is over all unit cells), P the pitch, $*$ signifies convolution, and A is the repeating area of the 2D profile (i.e., the unit cell). Interfacial roughness was incorporated into the model using the Debye-Waller factor (DW):

$$I(q) = I_0(q) e^{-q^2 DW^2} \quad (14)$$

The shape function for each line was a stack of six asymmetric trapezoids (Fig. 6). The expected shape was a repeating set of four asymmetric line profiles where the lines came in mirrored pairs (1-2 and 3-4). To account for this, the stacks were mirrored within each of two pairs. The shape of each

FIG. 7. Line geometry parameterizations for MBL-SEM libraries.

individual pair was defined by the same parameter set, but mirrored with a variable offset parameter. The parameters of a trapezoid in pair 1-2 were independent of parameters of the corresponding trapezoid in pair 3-4.

The model was fit to 1D slices in both the q_x and q_z directions of the experimental 2D scattering map. The fit optimization and uncertainty analysis used a Monte Carlo Markov Chain (MCMC) algorithm with a Metropolis-Hastings sampler as reported previously.[53-55] The method randomly varies the parameters around the best fit and determines the sensitivity of the model to the data. Uncertainties reported are the 95% confidence intervals of the accepted solutions.

5. Simulations and Fitting

In our initial MBL-SEM geometrical model, the lines were approximated as having trapezoidal cross-sections. Each trapezoid was characterized by 5 parameters: w_{Top} , θ_B , θ_A or θ_C , x_c (Fig. 7a), and h , respectively the width of the top of the line, the angles of its two sidewalls, its position (center top), and its height. Later, when this shape failed to adequately fit the data, we added a radius on one corner, as shown in Fig. 7b. In our most general library, we also allowed for the possibility of stray beam tilt [56] with a parameter, θ_t , that is the angular difference between the surface normal and the direction of incidence (as indicated by the arrows in Fig. 7b).

In simulations to build the library, the sample consists of lines, one centered ($x_c = 0$) and one on each side at separations (center to center) p_A and p_B . Inclusion of the neighboring lines allows the simulation to account for proximity effects, in which electrons escaping the sample near one line are intercepted by a neighbor. The neighboring lines are

assigned the same shape parameter values, but they are mirrored (left to right) with respect to the center line. The mirroring ensures that facing edges are similar, as expected from the symmetry (Fig. 4).

Crude estimates of most of the parameters were obtained by inspection of the image. Simulations were performed at discrete intervals along a range of values centered on this estimate. Parameters that were varied for library formation are shown in Table 1. For each of the 27000 combinations of the parameter values, a line-scan with at least 18000 simulated incident electrons at each x from -15.5 nm to 15.5 nm at 0.62 nm intervals was simulated.

For all materials, elastic scattering was modeled with the hybrid model described at the end of Sec. 3.2. In the SiO_2 lines, inelastic scattering mechanisms were SE generation via a DFT model (Sec. 3.3.1) and phonon scattering (Sec. 3.4). These models automatically account for energy losses, so no separate CSD stopping power model was required. In the Si_3N_4 outermost substrate layer, scattering tables for a DFT model were not available so SE generation was modeled by the fitted inelastic model (Sec. 3.3.2), coupled with the JoyLuoNieminenCSD stopping power model (Sec. 3.7). In both the lines and Si_3N_4 layer, electrons were tracked until they either escaped the sample and were detected or their energies fell below the barrier height, at which point escape from the sample becomes impossible. The remaining layers of the sample (TiN, SiO_2 , and Si) have no surfaces closer than 25 nm to the vacuum. From such layers, low-energy electrons have insufficient range to escape, so simulation time was conserved by dropping electrons with energy less than 50 eV from the simulation. Slowing down of the remaining higher energy electrons was modeled by either JoyLuoNieminenCSD (in the case of TiN and Si) or DFT (in the case of SiO_2), a choice dictated by convenience since these models agree at high energy (Fig. 3). All material boundary crossings were modeled as in Sec. 3.6 in the classical limit. The simulator's detector was set to return the conventional SE yield, i.e., the ratio of the number of electrons with energy less than 50 eV that reached the "chamber" (at considerable distance from the sample) to the number of

Table 1. Parameter values simulated for the library

Parameter	Description	Values	Unit
w_T	top width	7, 10, 12, 14, 17	nm
θ_A or θ_C	wall angle A- or C-side	0, 5, 10, 15, 20	°
θ_B	wall angle B-side	0, 2, 4, 8, 12, 20	°
r	corner radius	0, 6, 12	nm
p_A or p_C	separation A- or C-side	20, 25, 30, 35	nm
p_B	separation B-side	33, 38, 43	nm
θ_t	Stray beam tilt	$-3.4, -1.7, 0, 1.7, 3.4$	°

FIG. 8. Example simulation results. (a) Electron trajectories for one of the simulated geometries. (b) Simulated SE intensity profiles for two lines, identical to the ones drawn in (a) except for their widths: 10 nm and 12 nm.

incident electrons. At the high incident electron energies that were employed for imaging, the primary electrons penetrate well below the conducting TiN layer. Under this condition electron beam induced conductivity[57,58] may permit charge flows that equalize the charge distribution and minimize charge-induced contrast. We tried fits without charging on the hypothesis that such effects would avoid the need for time-consuming charging simulations. The resulting libraries fit the measured images well (See Sec. 6), so charging simulations were not done on this sample.

Fig. 8a shows electron trajectories at one landing position in a typical simulation. The beam was Gaussian with 0.31 nm (half pixel) standard deviation. This is large enough so that incident electrons produce a reasonable average over the whole pixel. Simulated results for larger beam sizes are produced by convolving the resulting intensity profile with a Gaussian of the desired width. Intensity profiles for rectangular lines of two different widths are shown in Fig. 8b. The intensity difference at mid-line ($x = 0$ nm) is not seen in wider lines, for which the intensity decreases to a steady minimum with sufficient distance from the edges.

The overall model function has this form:

$$M(x;p) = b + sL(x-x_0; \theta_t, w_T, \theta_B, \theta_A, r, p_B, p_A) * \frac{1}{\sigma_b \sqrt{2\pi}} e^{-\frac{x^2}{2\sigma_b^2}} \quad (15)$$

where $\mathbf{p} = \{s, b, \sigma_b, \theta_i, x_0, w_T, \theta_B, \theta_A, r, p_B, p_A\}$ is a shorthand on the left for the parameters listed explicitly on the right. The first four parameters in the list are instrument parameters: a scale (s) and offset (b) that define a linear relationship between yield as computed by the simulation and intensity as measured in the instrument, a beam landing spot size characterized by its standard deviation (σ_b), and a tilt angle (θ_i) equal to the deviation of the beam from the expected normal angle of incidence. The remaining parameters pertain to sample shape. In $L(x; \theta_i, w_T, \theta_B, \theta_A, r, p_B, p_A)$, all the parameters are the ones that are varied to build the library database. They are described in Table 1. The function L interpolates this library to produce curves like those in Fig. 8b. The parameter x_0 in Eq. (15) simply offsets the curve to the right or left, centering the line on x_0 instead of 0. The * signifies convolution of the curve with the indicated Gaussian to account for beam sizes larger than the one used in the raw simulations.

Given a measured image and its uncertainty, $I(x_i) \pm \sigma_i$, and parameter values, $\mathbf{p}$, we measure goodness of fit via

$$\chi^2 = \sum_i \left[\frac{I(x_i) - M(x_i; \mathbf{p})}{\sigma_i} \right]^2. \quad (16)$$

Starting from an initial guess, parameter values, $\mathbf{p}$, are adjusted according to the method of Levenberg and Marquardt[59] to minimize χ^2 . However, not all components of $\mathbf{p}$ are varied in the same way. p_A and p_B are library parameters that represent the distance between a line and its neighbors. These are needed to account for proximity effects: the reduced intensity at an edge with a nearby neighboring line due to the increased likelihood that electrons escaping from such an edge will be recaptured by the neighbor. This effect accounts for the different intensities of otherwise similar left and right edges in Fig. 8b. Such parameters are needed because the sample has trenches of varying widths (Fig. 5). However, the dependence is weak. Consequently, these parameters can be safely fixed at values determined from the image, and are not varied during the fit. The instrument parameters should be the same for an entire image. Consequently, fitting is performed in two steps. In the first step, a sample of three lines chosen in each of four linescans distributed across the image are fit. Each of the lines has its own

FIG. 9. Median fit (continuous curve). The error bars are ± 2 standard deviations of image noise. The inner and outer pairs of vertical lines mark the top and bottom corner assignments respectively.

geometrical parameter values, but the four instrument parameters are the same. The above fit is repeated eight times with different sampled linescans and lines. Mean values of the instrument parameters and their uncertainties are determined from the results. Finally, with instrument parameters pinned to the values thereby determined, in the second step each of the 14 lines (omitting the outermost two lines in Fig. 5) in each of the 421 line-scans was fit independently, floating only its own geometrical parameters. The above process was repeated for each of the four images.

6. Results

6.1 Fit results

The median (50th percentile) fit from the image in Fig. 5 is shown in Fig. 9. If the observed image noise (vertical error bars) accounted for all fit imperfections, χ^2 would be approximately equal to the number of degrees of freedom, ν . In fact, $\chi^2/\nu \approx 1.26$, so about 12% ($\sqrt{1.26} - 1$) of the observed residual must be due to other errors. Nearer the extremes, the 10th and 90th percentile fits have $\chi^2/\nu \approx 2.6$ and ≈ 0.61 respectively.

FIG. 10. Fit residuals: absolute value of the difference between measured and modeled images, shown at the same gray scale as the image in Fig. 5. (a) Trapezoidal model with normal beam incidence. (b) Rounded corner model with normal incidence. (c) Rounded corner model with stray beam tilt.

Table 2. MBL-SEM parameters of mean unit cell

Parameter	Line 1	Line 2	Line 3	Line 4
x_c (nm)	15	39.0 ± 0.6	76.7 ± 1.3	106.8 ± 1.8
w_T (nm)	11.0 ± 0.4	11.2 ± 0.4	10.3 ± 0.5	10.4 ± 0.3
θ_B ($^\circ$)	4 ± 1	2 ± 1	3.2 ± 0.9	0.8 ± 0.8
θ_A ($^\circ$)	3.6 ± 1.4	4.4 ± 0.8		
θ_C ($^\circ$)			5 ± 1	8 ± 1
r (nm)	8 ± 2	7.3 ± 0.8	9 ± 3	6 ± 1

The simulated library used for Fig. 9 was the best-fitting of three. The first attempt (Fig. 7a) was the simplest. The beam was normally incident ($\theta_t = 0$) and top corners unrounded ($r = 0$). The magnitude of the residuals is shown in Fig. 10a. The median χ^2/ν was approximately 2. The simulated intensity systematically exceeded the measured intensity at the line edges that faced each other across the A and C trenches, fabrication of which differs from the B trenches. (See Fig. 4.)

The excess brightness at A and C edges motivated the introduction of rounded top corners on those edges, as in Fig. 7b. With this change, χ^2/ν improved to approximately 1.5 with residuals shown in Fig. 10b. Edges in this new fit exhibited a left/right asymmetry: facing A edges had different average radii and sidewall angles. The same was true of facing C edges. The assigned geometrical differences correspond to actual observed differences in the average brightness of left-facing and right-facing edges. The observation could be due to a geometrical difference, as assigned by this fitting procedure. However, this is unexpected since the fabrication process treats these edges the same. An alternative explanation is possible: perhaps the sample or beam[56] was slightly tilted. Considering this possibility, the final fit, of which Fig. 9 is an example, included θ_t as an additional floating instrument parameter. The best fit had $\theta_t = -1.85^\circ$, still smaller residuals (Fig. 10c), and $\chi^2/\nu \approx 1.26$. Some geometrical left/right asymmetry remained in this best fit, though smaller than in the previous one.

These fits determine the values for a large number of parameters: The image in Fig. 5 consists of 421 linescans. Each linescan has 14 lines. Each of these lines is described by 5 shape parameters (center position, top width, two edge angles, and a radius). This represents a total of 29470 parameters from the image.

In each of the individual fits, the noise (represented by the error bars in Fig. 9) affects the repeatability of the parameter value determinations. These repeatabilities are estimated by the usual procedure, as diagonal elements of the covariance matrix. (See, e.g., Bevington and Robinson[60] p. 122.) The median individual fitting repeatabilities for parameters x_c , w_T , θ_B , θ_A or θ_C , and r for the image in Fig. 5 were approximately 0.1 nm, 0.2 nm, 0.4° , 0.7° , and 2.6 nm respectively. The repeatability for corner radius is about a factor of 10 poorer than the other dimensional repeatabilities. This reflects a lower sensitivity of the SEM to radius: a change in

radius causes a relatively small change in measured intensity, which is then strongly affected by intensity noise, whereas a change in width makes a lateral shift of a steep part of the intensity curve, consequently a large intensity change at the edge position and much lower sensitivity to intensity noise.

6.2 Results for mean shape; comparison to CD-SAXS and TEM

Much of the information carried by the tens of thousands of individual parameter values pertains to variation of line position and shape across the field of view, but the parameters can also be averaged in order to compare the result to area-averaging methods like CD-SAXS, which determine parameters of the mean unit cell. The average repeat distance (unit cell size) was 129.6 nm with 1% standard uncertainty due almost entirely to the SEM's scale uncertainty. It could be reduced in future measurements by more careful scale calibration. The parameter values averaged over the 4 measured sites are given in Table 2. The four columns in the table correspond to the 4 lines in each unit cell. We defined the coordinates such that the center of the first line was at $x = 15$ nm. The given uncertainties combine 3.18 standard deviations of the means with scale uncertainty in order to represent 95% confidence intervals for included errors. (The 3.18 comes from Student's t table for 3 degrees of freedom.) The uncertainties include the effects of errors introduced by noise, instrument parameters (since stray tilt, beam size, and other parameters are altered by moving and refocusing, and therefore were refit from the beginning), site to site variation in the sample, and the 1% scale uncertainty. Although the effect of noise is included, a benefit of averaging so many individual fits is that its effect on these values is far smaller than the individual fit repeatabilities discussed in the previous paragraph. In fact, the noise contribution is negligible, and the uncertainties of most parameters in Table 2 are dominated by line shape roughness within the individual images and site to site variation among images. The exception is for x_c for which some values were close to 100 nm and for which therefore the 1% scale error becomes important. (The other contributors to x_c uncertainty amount typically to 0.3 nm.) The tabulated values include contributions only from known sources of error. They omit contributions due to errors in the geometrical or physics model. These will be discussed in Sec. 6.4.

A cross-section of the unit cell described by the Table 2 parameter values is shown in Fig. 11a, where it is compared to the CD-SAXS mean unit cell. The CD-SAXS unit cell size was 128.7 nm, with 1% standard uncertainty. The MBL-SEM and CD-SAXS values differ by less than 1 nm, well within the uncertainty. Both are model-based techniques. In this case the assumed geometrical models differ in some respects, reflecting the different sensitivities and capabilities of the methods. The CD-SAXS model permitted some broadening of the line at the bottom, to account for line

FIG. 11. Comparison of shape assignments for MBL-SEM vs. (a) CD-SAXS and (b) cross-sectional TEM. The SEM result is the smooth curve (blue on-line) with rounded corners while the CD-SAXS result in (a) consists of joined line segments.

“footing.” The MBL-SEM model omitted this because the reduced signal from the bottoms of the trenches did not seem to warrant additional free parameters. The MBL-SEM corner model was rounded, whereas the CD-SAXS analysis presently requires piecewise linearity, so used two trapezoids to approximate the rounding. The CD-SAXS model imposed left/right reflection symmetry, requiring the shapes within the 1-2 and 3-4 pairs (see Fig. 11 for line numbering) to be mirror images. The MBL-SEM model did not impose this condition because even were it true on average, individual profiles (which the SEM resolves) may exhibit random deviations from symmetry.

In Fig. 11b the MBL-SEM result is compared to a TEM cross-section of a line array taken from an adjacent column. The lines numbered 1 through 4 correspond to the same unit cell choice made when computing the average given in Table 2. Those labeled 1' through 4' are their periodic equivalents. As with the CD-SAXS comparison, MBL-SEM and TEM agree qualitatively well on aspects of the line shape, for example that corners facing across A and C gaps are rounded with larger edge slopes while edges facing across B gaps are steeper and unrounded. In making comparisons, it is necessary to remember that the MBL-SEM result is an average over four $508 \text{ nm} \times 418 \text{ nm}$ areas whereas the TEM image is a much more limited sample within which there is evident variation. For example, line 3 leans to the left much more than its periodic equivalent 3', and lines 1 and 2 have less corner rounding than 1' and 2'.

To go beyond the qualitative resemblance among the results and quantify differences in widths and sidewall angles determined by the different methods, TEM values for widths and angles were determined based on profiles digitized from the image at the intensity approximately midway between the lines and their background. We begin with line 3, where the differences are largest. Angles θ_B and θ_C differ from both the CD-SAXS and MBL-SEM values by 3° to 7° . As mentioned above, this line also differs significantly from

Table 3. Comparison of MBL-SEM, TEM, and CD-SAXS parameter values averaged over the unit cell, omitting line 3.

Method	w_{mid} (nm)	θ_A ($^\circ$)	θ_B ($^\circ$)	θ_C ($^\circ$)
MBL-SEM	13.4 ± 0.2	4.0 ± 0.7	2.2 ± 0.4	8 ± 1
TEM	12.9 ± 0.3	7 ± 3	$0. \pm 2.$	8 ± 3
CD-SAXS	12.6 ± 0.3	$5. \pm 1$	-0.4 ± 0.6	7.8 ± 0.9

the partial TEM image of line 3'. Thus, even on strictly internal-to-TEM evidence, it is not clear that line 3 is representative. The remaining lines, 1, 2, and 4, have middle widths and angles (though not, as noted above, corner radii) that are consistent with their primed counterparts. The averages for these remaining lines are shown in Table 3. The middle width, w_{mid} (linewidth at half height), is compared to avoid complications from the different models and varying corner radii. For the SEM data, middle width is computed from the top width and sidewall angles as $w_{\text{mid}} = w_T + h([\tan(\theta_B) + \tan(\theta_{AC})]/2)$ with $\theta_{AC} = \theta_A$ for lines 1 and 2, θ_C for line 4. For the purpose of this comparison, the results of all tools were normalized to the same unit cell size. With relative scale errors thereby eliminated from the comparison, the stated uncertainties in Table 3 do not include a scale contribution. The MBL-SEM and TEM uncertainties represent the 95% confidence interval of the mean, as judged by observed variation over multiple unit cells. Those for CD-SAXS are estimated by the 95th percentile of the accepted solutions from a Monte Carlo Markov Chain method, as described in Sec. 4.2. The relatively higher TEM uncertainties were due to fewer measured locations to include in the average.

6.3 Results for shape variation

Model-based optical or x-ray methods determine an average geometry directly, from a model that relates the average geometry to the scattering signal derived from a relatively large illuminated area. In model-based SEM measurements, the SEM's native higher spatial resolution is retained; much of the information in the large determined parameter set relates to spatial variation of shape within the image. This is illustrated in Fig. 5, where some of the top and bottom edge assignments determined from these parameters are superimposed on the line edges.

Parameters from fits within Fig. 5's rectangular marked area were used to render the Fig. 12 3D representation. The sample was of good quality, with only small spatial variation. The top linewidth roughness was 1.2 nm to 2.4 nm (3 standard deviations), depending on line within the unit cell.

An earlier, lower quality sample that we used to develop our procedures contained some interesting defects that illustrate the usefulness of the SEM's locally resolved shape assignments. The inset of Fig. 13a shows an area where the MBL-SEM's bottom edge assignments cross. The corre-

FIG. 12. Part of a three-dimensional reconstruction from an image.

sponding assigned profile is shown in Fig. 13a. In Fig. 13b, a FIB cross-section shows one of these positions on the sample. Since we did not anticipate line overlap, the geometrical model's repertoire of possible shapes does not include anything quite like this shape. The assigned shape in Fig. 13a seems a reasonable approximation, within the limited repertoire of allowed shapes, of defects like the one in Fig. 13b.

6.4 Model errors

The fitting procedure finds only the best shape within a given parameterization family determined by the choice of

FIG. 13. Locally resolved defect information. (a) The best fit bottom edge positions crossed in a few places on an earlier sample. (b) SEM of a FIB (focused ion beam) milled cross-section indicated corresponding regions like this one, with incompletely etched lines.

geometrical parameterization. When the true shape does not belong to this family, there is necessarily some remaining error. In Sec. 6.1 we saw that the fits improved during two successive iterations in which the parameterization was improved. That bad geometries produce bad fits is as important as that good geometries produce good fits. This demonstrates that the technique has sensitivity. However, even the best parameterization found so far is not perfect. Any remaining imperfection is expected to lead to some bias in the measurement values.

Models may also err by making incorrect assumptions about material properties, by omitting important interaction mechanisms, or by incorrectly approximating interaction mechanisms that are included. Any of these can cause differences between the predicted and actual measured signal from a given shape. To the extent that the same model is used whenever a measurement with the technique is made, one expects similar errors: a bias. Such a bias would combine with the geometrical modeling error discussed above. A second, different, method would have its own bias. To the extent that two methods (e.g., SEM and optics- or x-ray-based) rely upon significantly different measurement principles, they share few physics assumptions, and their biases are independent. Differences in their biases are observable in measurement comparisons. This phenomenon is one source of “methods divergence,”[61,62] wherein different methods for quantifying the same measurand systematically produce different results.

As we will discuss and justify in the next section, errors associated with an incorrect choice of model are difficult to quantify. For this reason we have included no such uncertainty components in the totals in Table 2 or Table 3.

7. Discussion and Conclusions

To measure a quantity of interest (e.g., a width or angle) from a measured signal (e.g., an image or scattering pattern), we need a model that specifies the relationship between them. We also need to know how any other variable sample or instrument characteristics affect the signal. This is especially important when we need uncertainties near or below a microscope's spatial resolution, a requirement often faced for nanometer-scale objects, since we reasonably desire measurement uncertainties small compared to the objects we measure. At that point at least, if not earlier, metrology is limited by the availability and accuracy of models.

In this paper we have described JMONSEL, a model-based simulator designed for 3-dimensional length metrology with MBL-SEM (model-based library SEM), and tested it on a challenging state-of-the-art sample, a pitch-quartered array of lines with non-rectangular shape, top widths approaching 10 nm, and varying center-to-center spacings, the smallest of which was approximately 24 nm. In order for this to be a test of the model, the results must be compared to independent techniques, i.e., ones that rely upon different physical principles and therefore have as few model assump-

tions as possible in common with SEM. In this case the comparison was to TEM and CD-SAXS.

The model error discussed in Sec. 6.4 differs from that which is usually treated in statistics. Ordinarily one assumes that the form of the model function is known, and only some of its parameters are uncertain. In a one-dimensional example, the model, $M_1(p)$, is a known function. Perturbing the value of p from its best-fit value makes the predicted signal differ from the measured one, eventually by an amount that is inconsistent with the measurement uncertainty. A statistical analysis of the probability of a given mismatch allows the uncertainty in p to be quantified. In this way, mathematical or statistical considerations determine the uncertainty in p for a given model and data. Do strictly mathematical or statistical considerations likewise constrain how much p might be affected if the model had a different form, $M_2(p)$?

Elementary considerations are enough to convince oneself that the answer is no. If we are allowed to change the function, then among the possibilities is $M_2(p) = M_1(p - p_o)$. Here, p_o is some offset. If p_1 provides the best fit under model M_1 , then the best fit under model M_2 is $p_1 + p_o$, because $M_2(p_1 + p_o) = M_1(p_1)$. Thus the two models give fits of equal quality, but at parameter values that differ by p_o . This difference is unbounded; we can make it as large as we like with no loss of fit quality by choosing p_o appropriately. The existence of even one such example is sufficient to demonstrate that mathematical or statistical considerations like goodness of fit do not constrain the size of model-associated errors when the choice of model is not itself in some way further constrained. Any such further constraint is a matter of scientific judgment (e.g., consistency of the model with the best available theory).

The usual practice, and the one we have adopted, is a self-consistent approach. One initially assumes the model is correct, therefore includes no uncertainty component associated with any possible modeling error, and finally ascertains whether the measurement results are consistent with that initial assumption. In Table 3, the MBL-SEM and CD-SAXS middle widths differed by 0.8 nm. The difference is unlikely to be explained by the combined uncertainty of less than 0.4 nm. Rather, the result is consistent with a sub-nanometer relative bias between the two techniques, though the data give little guidance concerning how that bias should be apportioned between them.

The MBL-SEM and CD-SAXS estimates of the average linewidth at half the line's height differed by 0.8 nm, with the TEM value between them, 0.3 nm larger than the CD-SAXS value and 0.5 nm smaller than the SEM one. Based on the present comparison, we might estimate the magnitude of random biases among our techniques at around 0.4 nm (the standard deviation of our 3 widths). This is a crude estimate, suffering as it does from small sample size (only 3 techniques). Nevertheless, measurements performed with a single technique, as is commonly done, may have biases like these that remain entirely unrecognized. The sub-nanometer discrepancies in the present model-based measurements

compare favorably with previously observed differences of 10 nm or more between conventional SEM widths and corresponding atomic force microscope values.[63,64] The bias might be accounted for by errors in the shape parameterization, material properties, or model physics of MBL-SEM or CD-SAXS or both that have not yet been identified and included in the uncertainty estimates.

The three techniques were in good agreement concerning the composition (4 lines) of the repeating unit cell, the repeat distance, the spacings of lines within the unit cell, the general shapes of the lines (bottoms wider than tops, unequal left and right sidewall angles, significant rounding on one of the top corners), and the left/right alternation of line orientation. The sidewall angles mostly agreed within their uncertainties. The MBL-SEM and CD-SAXS estimates of the average linewidth at half the line's height differed by 0.8 nm, with the TEM value between them, 0.3 nm larger than the CD-SAXS value and 0.5 nm smaller than the SEM one.

Fits with three different libraries demonstrated that a library that includes stray beam tilt and corner rounding fit the data significantly better than libraries that did not, demonstrating that MBL-SEM has measurement sensitivity for these parameters. In distinction from other model-based measurement techniques, MBL-SEM retains the SEM's high spatial resolution. It is a local technique, which can measure pattern variation and detect individual defects.

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