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Dimensional Metrology of Resist Lines using a SEM Model-Based Library Approach

J. S. Villarrubia^a, A. E. Vladár^a, B. D. Bunday^b, M. Bishop^b ^aNational Institute of Standards and Technology,[†] Gaithersburg, MD, 20899 ^bInternational SEMATECH, Austin, TX 78741, USA

ABSTRACT

The widths of 284 lines in a 193 nm resist were measured by two methods and the results compared. One method was scanning electron microscopy (SEM) of cross-sections. The other was a model-based library (MBL) approach in which top-down CD-SEM line scans of structures are compared to a library of simulated line scans, each one of which corresponds to a well-defined sample structure. Feature edge shapes and locations are determined by matching measured to simulated images. This way of determining critical dimensions makes use of known physics of the interaction of the electron beam with the sample, thereby removing some of the ambiguity in sample edge positions that are assigned by more arbitrary methods. Thus far, MBL has shown promise on polycrystalline silicon samples [Villarrubia et al., Proc. SPIE 4689, pp. 304-312 (2002)]. Resist lines, though important in semiconductor manufacturing, pose a more difficult problem because resist tends to shrink and charge upon electron beam exposure. These phenomena are not well characterized, and hence are difficult to include in the models used to construct libraries. Differences between the techniques had a systematic component of 3.5 nm and a random component of about 5 nm. These differences are an upper bound on measurement errors attributable to resist properties, since they are partly attributable to other causes (e.g., linewidth roughness).

Keywords: critical dimension (CD); linewidth; model-based library metrology; resist; Scanning Electron Microscopy (SEM)

1. INTRODUCTION

A microscope image is an imperfect representation of the sample. High resolution scanning electron microscopy (SEM) is quite good, but the demands of accuracy placed upon it by the semiconductor industry are very high. At the nanometer and sub nanometer uncertainty levels being required for current and near-future device generations, important instrument artifacts must be accounted for in the measurement of feature widths. For width determinations with the SEM an important artifact is the edge bloom that results from electron scattering within the sample and secondary electron production by electrons scattered through a feature's steep sidewalls. The bloom is what creates the contrast that distinguishes edges from the rest of the sample, but the finite width of the bloom may create tens of nanometers of ambiguity in the edge position (Fig. 1). Existing CD-SEM (critical dimension SEM) edge finding algorithms make arbitrary assignments of edge positions. Such arbitrary assignments are made with the knowledge that they will produce a measurement bias (i.e., a nonrandom component of error) and with the hope that the bias will be consistent from sample to sample, thereby leaving measurements of width differences unaffected. The bias inherent in these methods of edge assignment is too large to meet the now very tight accuracy requirements in the ITRS.¹ Recent simulations² and experimental studies³ suggest that even the assumption of constant bias breaks down at the few nanometer level. The bias may vary from one sample to the next, with the result that commonly used algorithms may contribute several nanometers of error even to measurements that compare one width to another.

To do better requires that we know how the instrument interacts with the sample to produce the image. Such knowledge is embodied in a computational model of the probe-sample interaction—a piece of software that uses known or assumed physics of the interaction to calculate the image that would be observed for a given sample geometry.

With such a model in hand, it is possible to make a more reasonable assignment of edge positions. One such electron simulator is MONSEL, developed at the National Institute of Standards and Technology (NIST) in the 1990's.⁴ MONSEL

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uses Monte Carlo methods to simulate secondary electron production from linear features. In the last few years such instrument modeling has been applied to a case of particular interest to semiconductor manufacturers, SEM images of silicon lines.⁵⁻⁸ Cross-sectional profiles of actual polycrystalline Si ("polysilicon") lines or gates may differ in important ways from ideal rectangles. For example, corners may be rounded and sidewalls may not be perfectly vertical (Fig. 2). Determining as many of the shape parameters as possible, including of course the width, is the object of the MBL (model-based library) measurement algorithm developed during the course of these earlier studies.

The principle of operation of the MBL method is illustrated in Fig. 3. The unknown sample is imaged in the SEM. The measured intensity profile at each edge is then compared to a set of profiles previously calculated for a range of edge shapes using MONSEL. By interpolating between profiles in the library, the profile that best matches the measured edge profiles is found. The corresponding edge parameters are attributed to the unknown specimen.

In 2001, comparison of the MBL-determined profiles (based upon images obtained with a laboratory SEM at NIST) with the profiles measured in cross-section gave good agreement for the line's width and the angles of the side walls (Fig. 3a). Widths determined by regression to baseline were biased by approximately 15 nm and exhibited a more than a factor of 3 poorer repeatability.^{6,7} Similar measurements were repeated in 2002, but



FIG. 1. Edge assignment uncertainty: The finite width of the edge in a scanning electron microscope (SEM) profile of a line results in uncertainty concerning the proper edge assignment. The two rectangular lines beneath the image profile both have edges within the bloom regions and so are a priori equally plausible, but they differ in width by 10 nm.





FIG. 2. Parameterization of a UV resist line: Seven geometrical parameters and three instrument parameters are indicated. A BARC layer 80 nm thick was included between the wafer and the line.

FIG. 3. Schematic operation of model-based library measurement. The measured SEM signals from each edge of the unknown sample are compared to signals in the library to determine the parameters that produce the best match. (The library only contains right edges, which are reflected left to right when matching to measured left edges.) The parameters include some affecting edge shape in addition to edge positions, so some shape information is obtained from the image in addition to the CD.



FIG. 3. Application of MBL to polycrystalline Si samples. a: Edges (smooth wide trapezoid, red in color versions of this document) deduced from top-down image using the model-based library method compared to edges (thinner noisier line, blue) deduced from the cross section image on which both are overlaid. b: Example result of comparison of MBL determined cross section (smooth trapezoidal line on or near the Si-vacuum interface, light blue in color versions) determined from a CD-SEM top down measurement performed using a commercial CD-SEM at ISMT. The linescan from the CD-SEM measurement is shown in white. The profile determined from the top down measurement is overlaid on a cross section image measured later. As usual, the cross section may have missed the target location by a small amount, and this may account for the remaining small differences between the profiles.

using a commercial CD-SEM operated under fabrication facility conditions.⁸ An example of the agreement obtained is shown in Fig. 3b.

The materials of greatest industrial interest are polysilicon and various resists, polysilicon because the smallest critical features in the manufactured end product are polysilicon transistor gates and resist because measurements prior to etch (when the sample consists of resist on as yet unpatterned polysilicon) are used in process control. Polysilicon also has advantages for standards, because resist is dimensionally unstable, an important disadvantage in a dimensional standard. Because of this and because there are other problems in measuring resist, polysilicon samples were deemed more suitable test samples during development of the MBL method. For this reason, the studies referenced above all made use of polysilicon samples.

In this study we turn our attention to resist. Resist shrinks upon electron beam exposure. It is insulating, so accumulates charges that may affect the trajectories of subsequently produced secondary electrons. Certain of its properties (e.g., its plasmon resonance energy) that influence the secondary electron yield are only poorly known, making modeling it more uncertain. It was not known at the inception of this study whether these issues represented only annoyances or insurmountable obstacles to good CD (i.e., width) metrology. The general approach is similar to our previous studies of polysilicon samples. Resist samples were measured top-down in the CD-SEM. From these images, the sample cross-section was determined using the MBL method. These samples were cross-sectioned as close as possible to the area that had been imaged top-down. These cross-sections were imaged and the profiles determined from them. The widths determined by MBL were compared to the widths determined directly by cross-sectioning.

2. EXPERIMENTAL

The test pattern used for this project is shown schematically in Fig. 3b. This pattern is one of many on the AMAG4L reticle at International SEMATECH (ISMT). ISMT fabricated samples consisting of 290 nm tall developed Sumitomo PAR-810 resist lines on 80 nm of Brewer Science ARC29A in a focus-exposure matrix.⁹ Within this matrix, measurement targets were located at the positions shown in Fig. 4. Within each die, targets were located in the regions labeled A, C, and



FIG. 4. Measurement patterns were located in the numbered die of this focus-exposure matrix.

FIG. 5. Schematic of NIST 2120 test pattern on AMAG4L reticle. Measurement targets are inside of the red boxes.

E in Fig. 5, corresponding to 100 nm, 200 nm, and 350 nm lines respectively. Within each of these regions there were both low magnification and high magnification targets, as shown in Fig. 6.

The top-down images were acquired using a recent model CD-SEM at ISMT using a landing energy of 500 eV and a beam current of 10 pA. The high magnification areas imaged were predosed with a 1000 eV electron beam, 4.5 μ s of dwell time per pixel, with 1024 linescans of 960 pixels each. The purpose of predosing the sample was to pre-shrink the lines, thereby reducing shrinkage of the resist during subsequent images. The high magnification images were taken with 992 × 128 pixels, a beam current of 10 pA, and a pixel dwell time of 2.3 μ s. The imaged area was 2.69 μ m × 2.1 μ m. These parameters result in an image pixel that is about 6 times larger in the vertical dimension than in the horizontal. This was done to reduce the electron beam exposure as much as possible without compromising the instrument's resolution in the important direction perpendicular to the lines, which were oriented in the vertical direction as shown in Fig. 8.

The sample was cleaved as close as possible to the areas that had been imaged top-down. However, these areas were on the order of 2 μ m square as indicated above, and the areas indicated in Fig. 5 were far enough apart that it was not possible in general to cleave precisely through the imaged areas. This means the top-down information and cross-section information derive from slightly different parts of the same line, and may differ from one another due to linewidth roughness. This contributes to the uncertainty of the comparison, so the extent of linewidth roughness was assessed using the top-down images. The cross-section images were 2560 × 1920 pixels with a 2.56 μ m × 1.96 μ m field of view and 1 keV landing energy. A typical image is shown in Fig. 8.

3. ANALYSIS

3.1 Generation of Resist Libraries

MONSEL was used to simulate SEM images of resist lines at 500 eV landing energy. The edges were parameterized as shown in Fig. 2. We simulated all combinations of four radii (0 nm to 60 nm with a 20 nm increment), six angles (0° and 1° to 9° in 2° increments), five line separations (isolated, 100 nm, 200 nm, 300 nm, and 500 nm) and two secondary electron extraction efficiencies (0% and 100%). (CD-SEMs often use electric fields to extract secondary electrons. These fields deflect electron trajectories up and away from the sample, thereby allowing electrons to be counted that would otherwise have collided with the sample and been reabsorbed. This parameter is a measure of the efficiency of this process.)



FIG. 6. The 100 nm "A" area of the NIST 2120 test structure. There is a 2 μ m pitch calibratible scale pattern on the bottom. Above that the black line segments on left and right indicate the line along which the sample is to be cleaved. The measurement targets are along that line. The colored labels, lines, and boxes are not on the wafer. Small shaded (red) squares indicate the high magnification image targets. The larger shaded (blue) boxes are areas of the low magnification images.

Two of the input parameters required for the modeling, the densities of cured ARC29 and PAR810 resist, were apparently not well known, either by resist engineers at ISMT or by the manufacturer of the materials. For this reason ISMT sent cured thin films of these materials on wafers to NIST, where the film densities were measured using x-ray reflectivity.¹⁰ The resulting densities were 1.29 g/cm³ and 1.26 g/cm³ for ARC 29 and PAR 810 resist respectively.

3.2 Assignment of Edge Positions from Top-Down Images

Of the images attempted, there were 48 pairs for which both the top-down and the cross-section images of dense line areas were successful. On these 48 targets, there were a total of 284 lines. The number of lines in an image depended upon the line size. Samples had ten nominally 100 nm lines, five nominally 200 nm lines, or three nominally 350 nm lines, with space widths drawn the same as linewidths in each case. (In fact, lines after etch were narrower than their nominal values by about 35 nm, as we will see later.) Each of the top-down images in these pairs was analyzed using the MBL method. For the fits, the line separation parameter was pinned to approximate values determined directly from the images. (Since the separations are greater than 100 nm, an error of a few nanometers has little effect on the predicted image. This differs from the sidewall parameters, to which the image is quite sensitive.) A subset of linescans in each image was analyzed in a single fitting operation with both instrument and sample parameters free. The instrument parameters (beam size, contrast, brightness, and extraction efficiency) were pinned to the values determined from this fit. The remaining fits were performed one scan line at a time with only three free parameters per edge. These parameters were the edge position, side-wall angle, and top corner radius. The bottom edge positions determined by a typical fit are shown in yellow in Fig. 7. The



FIG. 7. Result of MBL analysis of a top-down image of nominally 100 nm lines. The lines coinciding with the brightest pixel near each edge (dark lines, red in color reproductions) were the initial estimates used as input to the MBL fitting algorithm. The algorithm reports the bottom edge position (second set of lines, outside of the first set, yellow in color versions) and sidewall angle.

linewidth roughness can be determined from these edge curves. It averaged about 3 nm (root mean square) for all lines, independently of linewidth.

3.3 Modeling and Edge Assignment for Cross-Section Images

To complete the comparison, edge positions must also be assigned to the cross-section images. These images are also subject to blooming at the edges, as is evident in Fig. 8. MONSEL is capable of modeling sample geometries that can be described by roughly trapezoidal lines on a one to three layer substrate. Fortunately, the cross-section geometry can be treated as a special case of such a sample, one in which the "line" is very tall and the three "substrate" layers are either of





FIG. 8. Typical low (left) and high (upper right) magnification images of nominally 100 nm lines. The images were acquired with rectangular pixels: linescan spacings were larger than pixel to pixel spacings within a line. As shown here the images have been stretched to compensate. The cross section image that corresponds to this sample is shown at the lower right.





FIG. 9. Cross section imaging geometry. The sample is oriented with the cleavage plane facing up. The usual top of the line (in the CD-SEM imaging geometry), the sidewall, and the substrate are labeled. The hourglass-shaped object is schematic of the SEM's electron beam impinging near the edge of the cleavage plane. Within MONSEL this geometry can be treated as though the cleavage plane is a line top, the sidewalls are vertical, and the line is now very tall. The absence of a substrate in the direction of the beam travel is treated by telling MONSEL the substrate is vacuum.

FIG. 10. The intensity near a tall vertical edge depends upon the beam divergence angle. The three curves are labeled with the beam divergence angle in degrees. As shown here, if the angle is between 0° and 0.8° the point of maximum intensity may be anywhere from 3 nm to the left of the maximum to 5 nm to the right.

0 thickness or comprised of vacuum (Fig. 9). This was simulated in MONSEL for incident electrons at 1 keV, the energy for the cross-section images, and with beam cone angles varying from 0° to 0.8°. Corner radii and sidewall angles were zero, because this is what we expect for the cross-section geometry. In principle, the edge positions of the cross-section image might have been determined by fitting the observed profiles to this simplified library. However, as can be seen in Fig. 8, there was an artifact near the base of the lines in the cross-section images that manifested itself as a bright region adjacent to the line edges. This artifact is most likely some out-of-focus structure near the end of the line, several micrometers below the cleavage plane. It is visible in the image because of the SEM's large depth of field. Unfortunately, this structure complicates fitting a library profile to the measured profile. Instead, we determined the position of maximum intensity from the cross section image, and then added to this an offset in order to assign the edge position. The offset associated with various beam cone angles was determined by the modeling already described, and is shown in Fig. 10. As is evident in that figure, the offset from the maximum brightness to the true edge position (i.e., the position of the peak of each of the curves relative 0 on the horizontal axis) is a sensitive function of the beam cone angle. The shape of the cross-section SEM profiles near the line tops, where the influence of the previously mentioned artifact near the base was minimal, was most consistent with a beam divergence half angle of about 0.2° . At this beam half angle, the true edge position is slightly less than 1 nm away from the position of maximum bloom brightness, in the direction away from the line center. This was the offset we used to assign edge positions to the cross-section images. However, because of the sensitivity of the assignment to beam divergence, there is a substantial amount of uncertainty associated with this. If we assume the true divergence angle lies between 0° and 0.8° , then the offset, which we have taken to be approximately 1 nm, might lie anywhere between -3 nm and +5 nm. The sensitivity in cross-section images is much greater than for top-down images because the effective height of the line is so much larger (Fig. 9). When the beam diverges, parts of it still strike the sidewall even when the central beam position is considerably beyond the edge. This is unlike the situation in a top-view. In



FIG. 11. Comparison of edge positions assigned by the MBL method on the basis of top-down CD-SEM images (smooth red lines) with those assigned to the cross section image (noisier blue lines). The middle image (b) represents a typical match (i.e., 50^{th} percentile for goodness of fit). Half the time, agreement was better than this, and half the time it was worse. The top image (a) is at the 90^{th} percentile. (Only 10% of matches were closer.) The bottom image (c) shows one of the poorer matches—90% of the time agreement was better than this.

that view, the substrate is only a few hundred nanometers below the top surface where it can intercept all of the electrons as soon as the beam is aimed a few nanometers beyond the edge.

3.4 Comparison of MBL and Cross-Section Results

The result of each of the edge position determinations described above is a set of data describing the edges in each image. The MBL parameters include the position where each edge intersects the substrate and the angle of the edge. From these parameters a profile for that line was computed. To compare the MBL-derived profiles to the cross-section ones, it is necessary to compensate for any magnification difference between the CD-SEM and laboratory SEM tools. Since our samples are periodic arrays of lines, this was done by scaling one of the images until the periodicity of the lines was the same as that in the other image. (The result of this operation indicated that the CD-SEM and laboratory SEM scale calibrations differed from one another by 0.8%. This difference was consistent across all of the periodic image pairs.) After putting the results on the same scale, the profiles were shifted with respect to one another in the *y* direction in order to make the positions of the top of the substrate match, and in the *x* direction by an amount determined to produce the best fit between the two.

Three of the 48 such comparisons are shown in Fig. 11. With the goodness of fit judged by the sum of squares of the differences between the edge locations, these three represent a good fit (90^{th} percentile), the median fit (50^{th} percentile), and a bad fit (10^{th} percentile) in order to convey both the typical agreement and the amount of variation around that typical result. All of the examples shown here were taken from the nominally 100 nm features (which were actually approximately 69 nm after developing). However, the results for the wider lines (nominally 200 nm and 350 nm) were similar.

Quantitatively, the extent of agreement can be judged by determining the average top to bottom width of each line from the MBL results and from the cross-section images. We begin by computing a set of residuals, $\Delta w_i = w_{\text{MBL}i} - w_{xsi}$. The *i*th residual is the difference between the MBL result and the cross section result for the *i*th line. The 48 targets each had multiple lines, resulting in 284 residual values in all. The average residual was 3.5 nm, as shown in the third column of Table 1. This offset indicates that one or the other method (or a combination of both) has this much measurement bias. At the scale of our images, this bias amounts to approximately 1 image pixel on each edge of a line. There are two quite plausible sources of measurement bias that could account for this much difference. The first is error associated with the beam divergence angle. (Recall the discussion associated with Fig. 9.) The second is shrinkage of the resist due to electron beam exposure, a known phenomenon.^{11,12} Notice that the MBL result is systematically larger than the cross-section result (i.e., the table entries are positive). This difference has the correct sign: the cross-section images were taken after the MBL top-down images and were therefore subjected to an additional e-beam exposure, any shrinkage from which would tend to make them narrower than the MBL result. Either of these effects could easily account for the observed difference.

In addition to the measurement bias just described, there is also a random difference between the two determinations. That is, the difference between the MBL and cross section results for a particular line might be more or less than the average difference discussed in the last paragraph. The standard deviation of the residuals was about 5 nm, as shown in the last column of Table 1. In discussing the sources of this random error, it is convenient to divide it into two components.

One component is the variance within each cross-section image (i.e., within-target). In Fig. 11b, for example, there are ten lines, each of which has an associated residual. The standard deviation of these was close to 3 nm for all the different width targets, as can be seen in the table's 4th column. This variation can be understood in terms of the linewidth roughness (LWR). The cross-section represents a particular slice through the line. The width there is expected to differ from the average width by an amount characterized by the LWR. We measured the standard deviation in linewidth on these samples from the top-down images to be 2.9 nm. We therefore expect 2.9 nm of variation from this source, an amount that corresponds quite closely to the observed value.

This component of variance does not capture all of the variation because the standard deviations are computed with respect to each target's own average residual. These within-target averages vary from one target to the next. Since there is within-target variation, a certain amount of target to target variation is expected simply due to sampling, but such variation should be smaller by a factor of $\sqrt{3}$ to $\sqrt{10}$ since there are 3 to 10 lines within each image. Since the within-target variation is only about 3 nm, this is 1 nm to 1.7 nm, not large enough to explain the roughly 4 nm of variation observed and reported in column 5 of Table 1. The source of this variation remains somewhat mysterious. It is not a truly systematic error (as a faulty assumption about the instrument's beam divergence would be for example) because it is not the same for all targets. Neither is it completely random, since it would then show up in the within-target component. Rather, it is a systematic component that is associated with individual targets and varies from target to target. Some possible sources of variation that would behave this way include: 1) Target to target variations in the amount of charging or resist shrinkage due to inconsistent exposure of the targets during set-up and focusing. (This is possible since the cross-section image

			Random Error (nm)		
Nominal Linewidth (nm)	Actual Linewidth (nm)	Average w _{MBL} - w _{xs} (nm)	σ (within target)	σ (target to target)	σ (total)
100	62.1	3.2	2.6	3.2	4.1
200	166.6	4.0	3.2	5.5	6.2
350	316.7	3.3	3.7	4.0	4.7
All lines	—	3.5	3.2	4.4	4.9

 TABLE 1. Agreement between MBL and Cross-Section Results

acquisition in the ISMT FA lab is a manual procedure.) 2) Target to target variation in focus. The entire image is acquired at a single focus setting, but when the sample is changed the instrument must be refocused. MBL is meant to compensate for focus variation in the top-down images, but this would not apply to the cross-section images. 3) Since the top-down and cross section images were taken at different parts of the line, the possibility the lines all tend to be larger or smaller at the second location cannot be eliminated in principle, though it is not clear what would be the source of such correlation—perhaps local variations in the etch rate or optical effects.

4. CONCLUSIONS

The average linewidth of resist lines derived from top-down CD-SEM images using the model-based library (MBL) approach agreed with widths derived from cross-sections to within the uncertainty of the comparison. The difference of 3.5 nm (about 1 image pixel per edge) was within the margin of error determined principally by two components. These were 1) error in the cross-section edge assignment associated with the electron beam divergence angle (i.e., depth of field) being different from that which was assumed or 2) shrinkage of the resist due to electron beam exposure.

The sensitivity of the cross-section determination to the SEM's depth of field is a significant unexpected finding of this study. It represents a heretofore unappreciated error source for determining widths from SEM of sample cross-sections. This points to the need for the development of appropriate electron beam shape measurement methods.

There were random differences between the widths determined by the two techniques. This difference had a standard deviation of approximately 5 nm. Of this, 3 nm was expected due to linewidth roughness.

The effect of charging upon dimensional metrology has been a matter of concern when dealing with resist samples. The size of the effect has not been known, and the possibility that charging might render good model-based SEM metrology of resists difficult or impossible was a real one. It is possible that some of the unexplained random difference between MBL and cross section results, or some of the systematic difference between them, could be accounted for by effects due to charging or shrinkage. While some such effects cannot be ruled out, the size of the disagreement between MBL and cross-section measurements presented here places an upper bound of at most a few nanometers on the size of those effects. It is possible they were smaller than this, if other phenomena were responsible for these residual differences.

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