3-Dimensional Lineshape Metrology Using Small Angle X-ray Scattering

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Abstract. The need for sub-nanometer precision metrology of dense patterns for future technology nodes challenges current methods based on light scatterometry, scanning electron microscopy (SEM), and atomic force microscopy (AFM). We provide results of initial tests of a measurement technique based on small angle x-ray scattering (SAXS) capable of rapid measurements of test samples produced using conventional test masks without significant sample preparation. The sub-Angstrom wavelength provides nanometer level resolution, with the possibility of increased precision after further refinement of the technique. SAXS results are shown for a test photoresist grating at a variety of angles, demonstrating an ability to extract information on 3-dimensional pattern shape.

\section*{INTRODUCTION}

The precise measurement of feature shape continues to challenge existing metrology techniques as feature size decreases and feature density increases. The International Semiconductor Roadmap suggests sub-nanometer resolution is required to characterize gate and dynamic random access memory (DRAM) features within the next four years \cite{1}. Metrologies based on scanning electron microscopy (SEM) and atomic force microscopy (AFM) face challenges in the characterization of dense, high aspect ratio features \cite{2}. Light scatterometry (LS) has emerged as a viable alternative for current technology nodes, providing rapid non-destructive measurements of line width and shape \cite{3}. However, the wavelength employed in visible light techniques is currently more than an order of magnitude larger than common feature sizes, and further reductions in critical dimensions will begin to limit the level of detail probed by this technique.

In contrast to visible light, an x-ray based technique offers the possibility of probing with sub-Angstrom wavelengths. Using wavelengths smaller than the feature size, feature shape can be characterized using established methods of diffraction. The simplicity of models based on pattern diffraction offer the possibility of rapid, real time model fitting. In contrast, the complexity of LS models limits analysis to classes of pattern shapes obtained from extensive stored solution libraries.

In this publication, we describe efforts to develop a metrology technique for sub-100 nm pattern metrology based on small angle x-ray scattering (SAXS). Using results from a series of photoresist gratings, the technique provides nanometer level resolution of pitch and line width. The transmission geometry (see fig. 1) provides advantages in the simplicity of modeling and in the characterization of embedded structures such as in copper interconnects within a low-k matrix. The technique is demonstrated here using a synchrotron source, however the exportation to a laboratory scale device is feasible and discussed in more detail. A non-destructive probe allows precise measurement of samples without significant preparation or handling. Additional advantages include applicability to both organic and inorganic materials. Methods for extracting 3-D lineshape are outlined for patterns with well-defined material properties as well as systems with ill-defined properties.
**EXPERIMENTAL METHODS**

Test structures of photoresist gratings on silicon were created using three different photoresists (see fig. 2). Each pattern is imaged using optimal conditions for that resist. The nominal pattern consists of 180 nm lines with 1:2 spacing. Total area of the grating is approximately 1 cm².

Small angle x-ray scattering (SAXS) experiments were conducted at the ID9 Beamline of the Advanced Photon Source at Argonne National Laboratory. The wavelength, \( \lambda = 0.95 \ \text{Å} \), is selected using a single crystal monochromator. The resulting beam has a wavelength spread \( \Delta \lambda / \lambda = 3 \times 10^{-5} \). The beam size at the sample is controlled using a pair of focusing mirrors aligned along orthogonal axes and two rectangular slits. The resulting beam spot size is \( \approx [100 \times 100] \ \mu \text{m} \). A 2-D CCD detector is placed at a distance of \([543 \pm 2] \ \text{cm}\) from the sample [4].

**RESULTS AND DISCUSSION**

In figure 3, the detector image recorded for the “A” grating displays over 16 orders of observable diffraction peaks. The data were collected over a period of 5 min. Data of similar quality are obtained after only 10 s. The data collection time depends on many factors including incident flux, transmission of the sample, and beam spot size, and detector efficiency. The data of figure 3 illustrate the ability to extract relative pattern quality without the requirement of data modeling. For a given mask, the number of diffraction peaks is directly proportional to pattern quality. The loss of higher order peaks results from a wide range of pattern degradation indicators, including variations in line width and pitch. The evaluation of a dose-matrix is potentially achieved through counting the number of peaks produced by each element.

A 2-D detector provides information along the entire plane of the substrate. As a result, SAXS is capable of metrology of arbitrarily shaped patterns on 2-D lattices such as contact holes and via pads. Contact holes are especially difficult to characterize when measuring only 1-D due to the lack of planar sidewalls. In the case of a planar array of contact holes, SAXS potentially provides a detailed shape of the average contact hole including asymmetries.

In an effort to illustrate the capabilities of the technique, we provide a simplified analysis of pattern dimensions. We restrict the current discussion to data along the diffraction axis. In figure 4, SAXS intensities of all three samples are plotted as a function of the scattering vector \( q = 4\pi / \lambda \ \sin(\theta) \) where \( 2\theta \) is the scattering angle. The intensities from each sample, measured with the sample surface perpendicular to the direct beam, are plotted as a function of \( q \) in figure 3. The subtle differences observed in the SEM micrographs are apparent as variations in relative peak intensities in figure 4 (for example, see the 12\textsuperscript{th} order peak).

The repeat period, \( L \), of the pattern is inversely proportional to diffraction peak spacing \( \Delta q = 2\pi / L \). A linear fit of the peak intensity position as a function of peak order provides the periods for each sample as \( L = [553 \pm 1.8] \ \text{nm}, \ [550 \pm 2.2] \ \text{nm}, \) and

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**FIGURE 1.** Schematic of transmission scattering geometry employed by SAXS. Scattering angle, \( 2\theta \), is shown relative to the unscattered beam. Measurements at varying sample orientations are used to reconstruct 3-D lineshape, where the sample is rotated about the axis \( \omega \).

**FIGURE 2.** Scanning electron microscopy images of photoresist gratings. Patterns are constructed from three different photoresists (labeled A, B, and C) under optimal imaging conditions. Shown are cross sectional views (left) and top down views (right).
[543 ± 1.5] nm for the A, B, and C samples, respectively. Precision of pitch determination is limited by the number of observable peaks. In addition to pattern quality, measurable diffracted intensity at large q results from increased instrumental resolution. The conditions employed here are not optimized, allowing the possibility for future increases in instrumental resolution and information content.

Line shape parameters such as the average feature width are obtained from the relative intensities of the diffraction peaks. Approximating the cross section of the average line as rectangular, peak intensities are determined by the form \( I_{\text{peak}}(q) = A^2 |P(q)|^2 \), where A is an arbitrary constant and \( P(q) \) is the form factor of a line with rectangular cross section \( (\sin(qd/2))/q \) where d is the width of the line). A convolution with the instrumental resolution function provides the model fit in figure 4. Model fits of each sample yields values of the line width, \( d = [171 ± 1.2] \) nm, \( [159 ± 1.6] \) nm, and \( [167 ± 0.9] \) nm for A, B, and C respectively. In the case of sample C, the quality of the pattern results in sub-nanometer precision. As with periodicity, the uncertainty is dictated by the number of oscillations of the form factor observed within a measurement.

The calibration of intensity to absolute scale provides a potential to extract data along the 3-dimensional pattern. Intensity calibration is typically achieved by comparison to a standard sample of known electron density. The absolute scattered intensity measured from a pattern is a function of material composition, density, and pattern shape. The proportionality of absolute intensity and feature height allows the extraction of quantities such as line height and sidewall angle. The incorporation of absolute intensity is then a potential route to extracting information on the entire feature shape from a single measurement.

An alternative route to 3-dimensional characterization of line shape is possible when parameters such as pattern composition are not known precisely. The detector image of figure 3 is the fourier image of the real space projection of the grating on the surface of the Ewald sphere. Rotating the sample changes the projection axis analogous to tomography.

The sensitivity of SAXS to the 3-D line shape is demonstrated in figure 4. A model grating is constructed using dimensions similar to sample A. The projection of a perfect rectangular cross section is itself symmetric. Projections of trapezoidal cross sections are increasingly asymmetric as the sidewall slope decreases. In figure 4, theoretical SAXS intensity is shown for a series of gratings after projection along an axis 2° off normal incidence. The calculations vary the sidewall angle, or slope, while holding other parameters such as average line width, height, and pitch constant. A relatively small angle of rotation demonstrates the sensitivity of the form factor to sidewall angle. Given sufficient data quality, a detailed 3-D feature shape can be reconstructed from multiple projections. Collecting data from multiple sample orientations (see fig. 1) is therefore a viable route to 3-D pattern shape for patterns of unspecified composition.

The data presented here are collected using a synchrotron x-ray source, however application of the technique using a laboratory scale device is theoretically feasible. The transmission geometry makes the choice of wavelength key pattern metrology. As shown in figure 1, the beam must pass through nearly a millimeter of substrate to interact with the patterns, typically on the order of 500 nm in height. As a result, sub-angstrom wavelengths are employed to minimize absorption. However, decreased wavelength reduces resolution, where the
Theoretical SAXS intensities as a function of $q$ for a grating rotated 2º from normal incidence. Shown are predictions for a grating of dimensions similar to sample A with sidewall angles of 89.9º (top), 89.5º (middle), and 89.0º (bottom).

resolution, $\Delta q$, is approximated by $(\Delta q/q)^2 = (\Delta \lambda/\lambda)^2 + (\Delta \theta/\theta)^2$. At the current wavelength, the ratio of transmitted to adsorbed x-rays through a bare silicon wafer is $\approx 0.10$. The current wavelength is therefore a compromise, however it is not necessarily the optimal value.

Given the room for optimization, a laboratory-based SAXS tool is already feasible utilizing a bright x-ray source such as a rotating anode. In addition, we are currently exploring the feasibility of laboratory-scale devices based on commercial x-ray tube sources. Optical components used here including the monochromator, focusing mirrors, and 2-D detector are similar to components available from a variety of existing commercial sources.

CONCLUSIONS

We have demonstrated the capability of small angle x-ray scattering as a viable measurement tool for pattern characterization in sub-100 nm lithographic processing. The technique was demonstrated as applicable for both organic systems, such as in photoresists, and inorganic semiconductor structures. The technique currently provides nanometer level resolution, extendible to sub-nanometer levels with finer adjustments of x-ray optics. Finally, the sub-nanometer wavelength of the probe offers the possibility of model independent characterization of parameters such as periodicity and average feature width.

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REFERENCES

4. The data in this manuscript, in the figures, and in the tables are presented along with the standard uncertainty ($\pm$) involved in the measurement, where the uncertainty represents one standard deviation from the mean.