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Nanometrology using a through-focus scanning optical microscopy method

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Abstract
We present an initial review of a novel through-focus scanning optical microscopy (TSOM pronounced as ‘tee-som’) imaging method that produces nanometer-dimensional measurement sensitivity using a conventional bright-field optical microscope. In the TSOM method a target is scanned through the focus of an optical microscope, acquiring conventional optical images at different focal positions. The TSOM images are constructed using the through-focus optical images. A TSOM image is unique under given experimental conditions and is sensitive to changes in the dimensions of a target in a distinct way. We use this characteristic for nanoscale-dimensional metrology. This technique can be used to identify the dimension which is changing between two nanosized targets and to determine the dimensions using a library-matching method. This methodology has potential utility for a wide range of target geometries and application areas, including nanometrology, nanomanufacturing, defect analysis, inspection, process control and biotechnology.

Keywords: TSOM, through-focus, optical microscope, nanometrology, process control, nanomanufacturing, nanoparticles, overlay metrology, critical dimension, defect analysis, dimensional analysis, MEMS, NEMS

1. Introduction
The demand on tools to make measurements at the nanoscale is very high as dimensional information at the nanoscale is required to enable progress in nanotechnology and nanosciences [1, 2]. Several tools, such as the atomic force microscope (AFM), scanning tunneling microscope (STM) and scanning electron microscope (SEM), are routinely used to provide measurements at this scale. However, with the commercialization of nanotechnology, fast and reliable nanoscale feature measurements will become increasingly important [1, 2]. Optics-based tools can be advantageous because they have a relatively low cost of ownership with high throughput.

It is often a misconception that optical microscopes are not well suited for dimensional measurements of features that are smaller than half the wavelength of illumination (200 nm sized features in the visible region) due to diffraction [3]. It is true that diffraction-dominated images make meaningful analysis of the targets difficult. However, this limitation can be circumvented by (i) considering the image as a ‘signal’ that represents the target, (ii) using a set of through-focus images instead of one ‘best focus’ image and (iii) making use of highly developed optical models [4–6].

In conventional optical microscopy, it is usually deemed necessary to acquire images at the ‘best focus’ position for a meaningful analysis, based on the belief that the most faithful representation of the target is rendered only at the best focus position. However, the out-of-focus images do contain additional useful information regarding the target. This information may be obtained using an appropriate data acquisition and analysis method. Based on this, and on the observation of a distinct signature for different parametric variations, we introduced a new method for nanoscale-dimensional analysis with nanometer sensitivity for three-dimensional, nanosized targets using a conventional bright-field optical microscope [7–12]. The method is referred to as the ‘through-focus scanning optical microscopy’ (TSOM pronounced as ‘tee-som’) imaging method. The TSOM method has won R&D 100 award for the year 2010 [13, 14]. Here, we present an initial review of the TSOM method. The TSOM method is applicable to three-dimensional targets, thus...
enabling the method to be used for a range of target geometries and application areas.

In the following sections we present the methodology to construct TSOM images, the characteristics of the TSOM images, comparison of optical simulation to experiments and various applications for nanometer-scale-dimensional analysis. The experimental validation of nanoscale sensitivity using the TSOM method is also presented.

2. Method to construct a TSOM image

The TSOM method requires a conventional bright-field optical microscope with a digital camera to capture images and a motorized stage to move the target through the focus. In figure 1 we demonstrate the method to construct TSOM images using a spherical gold particle (typically encountered in medical applications [15]) as a target. Simulated optical images are used here to demonstrate the method. Optical images are acquired as the target is scanned through the focus of the microscope (along the Z-axis) as shown in figure 1(a). Each scan position results in a slightly different two-dimensional intensity image. The acquired optical images are stacked at their corresponding scan positions, creating a three-dimensional TSOM image, in which the X- and Y-axes represent the spatial position of the target, and the Z-axis the scanned focus position. In this 3D space, each location has a value corresponding to its optical intensity. The optical intensities in a plane (for example the XZ plane) passing through the location of interest on the target (through the center of the gold particle, for example) can be conveniently plotted as a 2D image resulting in a 2D-TSOM image as shown in figure 1(b), in which the X- and Y-axes, and the color scale (Z-axis) represent the spatial position of the target, the focus position and the optical intensity, respectively. For 3D targets, appropriate 2D-TSOM images are selected for dimensional analysis. The TSOM image in the current paper implied a 2D-TSOM image.

The TSOM images vary substantially for different types of targets. This variation is illustrated in figure 2 for four types of targets. A simulation of a reflection-based optical microscope measuring an isolated line is shown in figure 2(a). A finite dense array with nine lines produces the TSOM image shown in figure 2(b). This target has a pitch of 105 nm. In-chip overlay targets must be small so that they can be placed in the active area. The TSOM image of an in-chip target at $\lambda = 193$ nm is shown in figure 2(c). A TSOM image may also be produced for transmission microscopy; a photomask target in a transmission mode microscope at $\lambda = 365$ nm is shown in figure 2(d). This target has a chrome line on a quartz substrate.

To validate the simulation data, data were collected to produce an experimental TSOM image. For this experiment a Si line grating was chosen and the target and through-focus images were acquired at 100 nm through-focus step increments. Using reference metrology tools such as SEM and AFM the target bottom line width, the line height and the pitch were measured and found to be 152 nm, 230 nm and 601 nm, respectively. Using these as input parameters for the model, the simulated TSOM image was obtained. The experimental and the simulated TSOM images are presented in figure 3. Good agreement between the experiment and the simulation was observed, and the data from the figure are a demonstration of the validity of the TSOM imaging approach. In the next section applications of TSOM imaging for dimensional metrology are presented.

3. Two types of applications

At present, we propose two applications of the TSOM method:

(i) determination of a change in the relative dimension and (ii) determination of the absolute dimensions of a target.

The first type of application, sensitivity to dimensional change, requires a minimum of two targets. For sensitivity measurements, although simulations are not necessary, simulations greatly enhance the rigor of the method. The second type of application, determining the physical dimensions, requires accurate simulations. In addition, it also requires satisfactory experiment-to-simulation agreement for successful implementation. In the current work three types of
optical simulation programs were used [4–6]. The following is a detailed discussion of these two applications of the TSOM images.

3.1. Determination of a change in the relative dimension

A small change in the dimension of a target produces a corresponding change in the TSOM image. Comparing two TSOM images from different targets, one can identify that a change in the target dimension has occurred. Although one can compare and identify changes in different ways, here we present a method based on a differential TSOM image.

Although this method can be applied to any of the targets discussed in this paper, in the current analysis we demonstrate the approach for an isolated line (i.e. a line several wavelengths away from nearby features). The TSOM images were simulated for small changes in the target dimensions. In figure 4 we present TSOM images for two targets with a 1.0 nm difference in the line width. Visual inspection of the two TSOM images would indicate that they are similar.
Figure 4. The simulated TSOM images for two isolated line targets. LW = line width in nm, LH = line height in nm, illumination NA = 0.4, collection NA = 0.8, illumination wavelength = 546 nm, a Si line on a Si substrate.

Figure 5. The simulated differential TSOM images obtained for the isolated lines shown in figure 4. (a) 1.0 nm change in the line width, (b) 1.0 nm change in the line height, (c) 1.0 nm change in the line height and the line width and (d) 1° change in the sidewall angle (LW = line width in nm, LH = line height in nm).

In the same way, the TSOM images for a small change in the line height or the sidewall angle also appear similar. However, a simple subtraction of any two TSOM images distinctly highlights the difference between them. This difference may be illustrated using a differential TSOM image. The differential TSOM image is the difference in the optical intensities between any two similarly processed TSOM images. We analyzed the differential TSOM images for four different dimensional changes. They are a 1 nm change in the line height, a 1 nm change in the line width, a 1 nm change in the line width and the line height and a 1° change in the sidewall angle. The differential TSOM images for the four types of dimensional changes are shown in figure 5.

The following observations can be made from the differential TSOM images. For the simulations shown, it is possible to identify a small change in the dimension of the target using this method. However, sensitivity to small dimensional changes will depend on the measurement noise, sensitivity and the monotonic response. In the data it can be observed that a small change in the line height, the line width, both the line width and the line height, or the sidewall angle individually shows qualitatively distinct differential TSOM image responses. We have confirmed similar simulation-based results for several different types of targets. In figure 6 we present a second example for a finite dense line array at $\lambda = 193$ nm. Again we observe that the line height and the line width differences individually produce distinctive differential TSOM images. This simulation-based analysis demonstrates an intriguing possibility for identifying specific dimensions that have changed through the examination of differential TSOM images.

To validate how the simulation results compare to experiment we compare an experimental differential TSOM image, which includes noise and other experimental
imperfections, with the simulation analysis. We chose two line gratings (pitch = 601 nm) with 146 nm and 149 nm line widths (about 3 nm difference). Using $\lambda = 546$ nm light, we obtained two experimental TSOM images that yield one differential TSOM image. The process of obtaining the experimental differential TSOM image requires some explanation; we normalize the intensities of the experimental TSOM images such that the maximum intensity in the image is equal to 1 and the minimum intensity is equal to zero. The two normalized TSOM images are then cross-correlated to get the best match. At this point differential TSOM images are obtained. We applied the same normalization procedure to the simulation results to maintain consistency with the experiment. Differential TSOM images from the simulations and the experiments are shown in figure 7. Although agreement is far from ideal, the experimental and simulated differential TSOM images have substantial qualitative similarities.

As shown above, different dimensional changes (i.e. width or height) produce qualitatively distinct differential TSOM images. However, for different magnitude changes of the same dimension, the differential TSOM images appear qualitatively similar. In figures 8(a) and (b) we present the differential TSOM images for 2.0 nm and 4.0 nm differences in line width, respectively, for an isolated line. Similarly, we present the differential TSOM images for 2.0 nm and 4.0 nm differences in the line heights in figures 9(a) and (b), respectively, for an isolated line. These simulations yield qualitatively similar appearing differential TSOM images. We performed a similar analysis for several different types of targets under different conditions. In all the cases tested we observed a similar behavior. This behavior holds true as long as the difference in the dimensional magnitude is small compared to the dimension of the target. It is also important to note that the qualitative differences in the differential TSOM images for various dimensional changes (e.g. line width versus line height) are much stronger than compared with the differences observed in the differential TSOM images for various magnitudes of change in the same dimensional parameter (1 nm versus 2 nm line widths).

To quantify the magnitude of the difference for a single parameter, we evaluate the ‘mean square difference’ (MSD), which is defined here as

$$MSD = \frac{1}{n} \sum_{i=1}^{n} (\text{TSOM image}1 - \text{TSOM image}2)^2,$$

where $n$ is the total number of pixels in the image. 1.0 and 2.0 nm differences in the line widths of an isolated line (figure 8) produce the MSD values of $0.58 \times 10^{-6}$ and $2.45 \times 10^{-6}$, respectively. Similarly, 1.0 and 4.0 nm differences in the line heights, as shown in figure 9, produce the MSD values of $0.38 \times 10^{-6}$ and $1.56 \times 10^{-6}$, respectively. In these two examples, the MSD values increased in direct relationship to the magnitude of the dimensional differences. However, the amount of increase depends on the individual case. For consistent results and comparison, the total number of points in the images, the selected X-axis distance and the focus range must be kept constant.
3.2. Determination of the absolute dimension of a target

The utility of the TSOM image approach in metrology is based on an assumption that any given target produces a unique TSOM image under a given experimental condition. A preliminary test to study the uniqueness of the TSOM image using simulations found the assumption to be satisfactory [8].

We now apply the same technique to experimentally measure the line width of the line grating target shown in figure 3(b). These results are preliminary in nature. We evaluated the dimensions of the selected target, including the line width, using reference metrology tool such as an AFM. The AFM-measured line width was 145 nm for the selected target. However, in the analysis here we assumed the line width to be ‘unknown’. Using the measured dimensions we simulated a small library of TSOM images by keeping the line height (230 nm), the pitch (601 nm) and the sidewall angle (which is curved) constant. For the simulation of the library, we varied only the line width from 140 nm to 160 nm with a step increment of 0.5 nm. The library matching of the experimental TSOM image (figure 3(b)) was carried out by evaluating the MSD values from the differential TSOM images. The differential TSOM images between the experimental and the simulated TSOM images were obtained after they were aligned to get the best match. A plot of the MSD values thus evaluated as a function of the line width in the library is shown in figure 10. The inset shows a magnified view of the minimum of the curve. This gives the best line width match as 153 nm. The TSOM image-based line width value differs with the AFM-measured line width of 145 nm.

Figure 8. The simulated differential TSOM image obtained for (a) the line widths of 102 nm and 100 nm (2.0 nm difference) and (b) the line widths of 104 nm and 100 nm (4.0 nm difference). Isolated line, line height = 100 nm, illumination NA = 0.25, collection NA = 0.95, illumination wavelength = 546 nm, a Si line on a Si substrate.

Figure 9. The simulated differential TSOM image obtained for (a) line heights 102 nm and 100 nm (2.0 nm difference) and (b) line heights 104 nm and 100 nm (4.0 nm difference). Isolated line, line width = 100 nm, illumination NA = 0.25, collection NA = 0.95, illumination wavelength = 546 nm, a Si line on a Si substrate.

Figure 10. A plot of the MSD values evaluated comparing the experimental ‘unknown’ target with the library of simulations. The inset shows the magnified portion of the highlighted curve.

The discrepancy between the AFM and the optical technique used here requires further study and is beyond the scope of the current paper. However, this example demonstrates the potential utility of the TSOM method for absolute dimensional measurements.

4. Optimization

The sensitivity of a given measurement can be enhanced by optimizing experimental parameters such as polarization, wavelength, illumination and collection numerical apertures.
The polarization state of the illumination produces different sensitivities for a given dimensional difference. This is illustrated in [8] for an isolated line at $\lambda = 193$ nm and 100 nm nominal line height for unpolarized, TE-polarized (electric field pointing along the lines) and TM-polarized (electric field pointing perpendicular to the lines) illumination. The results show a large difference in the MSD value (i.e. sensitivity) depending on the illumination polarization for a 2.0 nm difference in the line height. Under the given simulation conditions, the TM polarization produced maximum sensitivity, about ten times the sensitivity compared with that of unpolarized light. Similarly one can optimize the experimental conditions such as illumination numerical aperture (NA) or collection NA to produce the maximum sensitivity [8].

5. Robustness to optical aberrations and process variations

For metrology applications it is important to evaluate the robustness of the differential TSOM image method. All optical tools have a degree of optical aberration. It is important to know the degree to which error is introduced in the measurement due to the presence of optical aberration. We studied this using simulations for the overlay measurement of an in-chip overlay target [11]. The TSOM images were simulated under two conditions: without optical aberration and with third-order spherical aberration (with the Zernike coefficient of 0.01). The optical intensity simulated with the programmed spherical aberration exhibited a considerable difference compared with the aberration-free profile. However, the evaluated MSD under the two conditions to measure the overlay showed a very small variation of about 0.0004 nm for a 4 nm overlay. The error in the overlay measurement is negligible under the experimental conditions indicating that this method is robust to optical aberration as long as the aberration remains constant between the compared TSOM images.

In practice, it is common to have process variations that produce small changes in the dimensions of the metrology targets, including overlay measurement targets [11]. For a 4 nm overlay the selected target in [11] produced the MSD value of $21.7 \times 10^{-6}$. A 5 nm change in the line height due to process variations produced the MSD value of $22.3 \times 10^{-6}$, which results in a 0.06 nm error in the overlay measurement. Similarly a 4 nm difference in the line width produced an overlay error of 0.032 nm. This example shows a relatively small error in the overlay measurement due to process variations, and hence makes this method robust for the example conditions studied in [11].

6. Optical models

For most of the simulation work presented here, a finite difference time domain (FDTD) optical model was used [5]. This model is capable of simulating 3D targets. On a limited basis a second, rigorous couple waveguide analysis (RCWA) optical model [4] was employed. The RCWA model is capable of simulating only 2D targets. 3D optical modeling is computationally intensive, and depending on the size of the simulation domain, grid size and accuracy required, a 3D simulation with FDTD model can take as little as a few hours to several days using a high-end desktop computer. The optical models used here have been thoroughly studied and compared in house to evaluate their accuracy.

In the current work, for the process-control-type applications, optical modeling may not be required as the method relies on differential TSOM imaging. However, the accuracy of the optical simulations is of paramount importance for the second type of application where an experimental TSOM image is compared with a library of simulations. A thorough quantification of the optical microscope such as illumination NA, collection NA, satisfactory Kohler illumination and uniformity of illumination across the field of view is also needed for this application. In addition, the optical constants of the target materials need to be determined precisely.

7. Some example applications

We highlight here some of the several applications that are possible with the TSOM imaging method.

7.1. Dimensional analysis of nanoparticles

In principle, the size and shape of nanoparticles can be analyzed using the TSOM method. Here we examine this application using simulations. First we present particle size analysis using the library-matching method. A typical TSOM image of a gold nanoparticle (60 nm) is shown in figure 1(b). The TSOM images for different sized nanoparticles change with size. We make use of this difference to determine the nanoparticle size. The first step for this is the simulation of a library of TSOM images for various sizes within the expected size range. In the second step we acquire the experimental TSOM images of the nanoparticle needing size determination. The third step is to compare the TSOM image of the nanoparticle of unknown size with that of the library to determine the MSD values of the differential images. A plot of the MSD values thus obtained is shown in figure 11. If the size of the unknown particle is within the size range of the library, in principle, the plot shows a well-defined minima. The size corresponding to the minima indicates the size of the unknown particle. In this example, an ‘unknown’ nanoparticle size of 69.5 nm produced the best-match size of 69.45 nm. An improved method is to create the library with the experimental TSOM images of the particles with pre-determined sizes. This nearly eliminates the issues arising due to mismatch between the simulated and the experimental TSOM images.

As presented in the above sections, one important characteristic of TSOM imaging is the ability to differentiate different dimensional changes. This is also applicable to nanoparticle analysis. We present here differential TSOM images for size and shape differences of nanoparticles. Figure 12(a) shows a differential TSOM image for a 2 nm difference in the size (diameter). Compare this with the
Figure 11. Determination of unknown particle diameter using the best-match method from a library of simulations. Library range: 60 nm to 80 nm. Best-match diameter: 69.45 nm. Illumination NA = 0.3, collection NA = 0.95, illumination wavelength = 365 nm, a gold particle on a quartz substrate.

differential TSOM image shown in figure 12(b) for a difference in the shape (ellipsoid to sphere). We can see that size difference has a distinct differential image compared with shape difference.

7.2. Defect analysis in gratings

Under certain circumstances a direct observation of the TSOM image is helpful. For example, the TSOM images can highlight the presence of defects and the type of defect in a dense grating. As a demonstration we present experimental TSOM images for six dense gratings (nominal pitch = 200 nm and nominal line width = 100 nm) fabricated with intentional defects as shown in figure 13. The six types of defects with 10 nm differences in the line widths produce distinctly different TSOM images, firstly indicating the presence of defects and secondly pointing to the type of defect. In contrast, the absence of defects would produce featureless TSOM images for these dense targets. This type of analysis is also applicable to isolated line defects in an array of lines as shown in figure 14 for 2 nm reduction in the line width, or several random defects present in a dense grating.

7.3. Overlay analysis

Target-specific overlay applications are demonstrated using simulation results at an illumination wavelength of 193 nm. The target is a finite dense array with nine lines. We present an analysis for an overlay offset of 2.0 nm of each alternate line. The differential TSOM image obtained using the base target (zero overlay offset) and the target with a 2.0 nm offset is shown in figure 15. The differential TSOM image shows good signal strength and sensitivity for a 2.0 nm overlay. A line is drawn in the differential TSOM image to indicate the center of the target. Positive or negative overlay values may be identified by analyzing the symmetry of the differential TSOM image about this center line. This type of target analysis has applications in double patterning lithography. For more information on application of the TSOM method for overlay analysis refer to [8] and [11].

8. Summary

This paper presents an initial review of a novel technique which uses the additional information contained in a set of through-focus optical images as compared with a single image at the best focus position. The two-dimensional TSOM method was used to analyze dimensional information of sub-100 nm targets. The TSOM images are formed by stacking the through-focus optical image intensity profiles such that the X-axis represents the lateral distance on the target, the Y-axis represents the through-focus position and the intensity of the image (the Z-axis) represents the optical intensity. We proposed two main applications of the TSOM images: (i) determination of a change in the relative dimension and (ii) determination of the absolute dimensions of a target. We presented several examples using the optical simulations and the experimental results.

Differential TSOM images are generally distinct for different parametric changes. They enable us to identify which parameter is different between the two targets. However, the differential TSOM images obtained for different magnitude changes of the same parameter appear qualitatively similar. In this case, the MSD value enables us to determine the magnitude of the difference in the dimension. The TSOM images enable us to determine the dimensions of an...
Figure 13. Experimental TSOM images for dense line gratings fabricated with intentional defects. Every (a) tenth, (b) fifth and (c) third line is smaller by 10 nm. Every (d) tenth, (e) fifth and (f) third line is larger by 10 nm. Illumination wavelength = 546 nm, nominal line width = 100 nm, nominal pitch = 200 nm, illumination NA = 0.36, imaging NA = 0.8.

Figure 14. The differential TSOM image showing the presence of a single line defect that is 2 nm smaller than the other line widths in a dense finite grating. LW = 35 nm, LH = 100 nm, pitch = 105 nm, illumination NA = 0.3, collection NA = 0.8, total number of lines simulated = 9, illumination wavelength = 193 nm, a Si line on a Si substrate.

Figure 15. The differential TSOM image application for double patterning overlay analysis showing an overlay offset of 2 nm for finite dense array. LW = 35 nm, LH = 100 nm, pitch = 105 nm, illumination NA = 0.3, collection NA = 0.8, total number of lines simulated = 9, illumination wavelength = 193 nm, a Si line on a Si substrate.

unknown target by the library-matching method, provided we have accurate simulations and experimental results for a fully characterized optical microscope. Potential applications of the TSOM method include defect analysis, inspection and process control, critical dimension (CD) metrology, photomask metrology, overlay registration metrology, nanoparticle metrology, film thickness metrology, 3D interconnect metrology (large range depth analysis such as TSVs) and line-edge roughness measurement. Numerous industries could benefit from the TSOM method—such as the semiconductor...
industry, MEMS, NEMS, biotechnology, nanomanufacturing, nanometrology and photonics. The method is relatively simple, inexpensive, has high throughput, provides nanoscale sensitivity for 3D measurements and potentially saves millions of dollars for nano/microscale metrology and manufacturing. Future work includes extending the current method to three-dimensional targets and analyzing the full 3D TSOM image space.

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