Faculty and Staff Publication:

Samuel O’Mullane, Brennan Peterson, Joseph Race, Nick Keller, and Alain C. Diebold

Citation for Article:


https://www.osapublishing.org/oe/abstract.cfm?uri=oe-22-21-26246
Enhancing one dimensional sensitivity with plasmonic coupling

Samuel O’Mullane,1 Brennan Peterson,2 Joseph Race,2 Nick Keller,2 and Alain C. Diebold

1 College of Nanoscale Science and Engineering, SUNY Pl, Albany, New York 12203, USA
2 Nanometrics Incorporated, Milpitas, California 95035, USA

Abstract: In this paper, we propose a cross-grating structure to enhance the critical dimension sensitivity of one dimensional nanometer scale metal gratings. Making use of the interaction between slight changes in refractive index and localized plasmons, we demonstrate sub-angstrom scale sensitivity in this structure. Compared to unaltered infinite metal gratings and truncated finite gratings, this cross-grating structure shows robust spectra dependent mostly on the dimension of the smaller line width and pitch. While typical scatterometry simulations show angstrom resolution at best, this structure has demonstrated picometer resolution. Due to the wide range of acceptable specifications, we expect experimental confirmation of such structures to soon follow.

© 2014 Optical Society of America

OCIS codes: (260.2130) Ellipsometry and polarimetry; (250.5403) Plasmonics.

References and links
1. Introduction

In the past decade, plasmons (the quasi-particle that describes coupling of light with a collective oscillation of electrons) have been used extensively for a wide variety of applications. Since structures can be tuned to excite plasmons when very specific conditions are met, one common use of plasmons is for nanoscale sensing of biological materials [1],[2]. Plasmons have also been used as sensors for material properties [3–5], as part of an alternative lithography method [6], and to boost performance of existing devices [7],[8].

This paper will focus on the design and simulated scatterometry of nanometer scale gratings that display extraordinary sensitivity due to plasmonic activity. In order to test the sensitivity to changes in the line width (critical dimensions) of the copper lines, the simulated grating structure is based on copper metal lines with a barrier layer between the copper and the dielectric. We will use an implementation of rigorous coupled wave analysis (RCWA) which has

Fig. 1. (a) Infinite grating. (b) Finite grating. (c) Infinite cross-grating. Grey is Si-substrate, white is oxide fill, gold is Cu grating.
already been used as an accurate simulation tool of non-destructive optical measurements of periodic grating structures [9], [10]. Additionally, there has been good agreement between RCWA and critical dimension (CD) measurements [11] and plasmon effects [12]. As will be shown, metallic gratings can be altered to produce distinct plasmonic peaks that enhance sensitivity to critical dimension. For comparison purposes, three structures will be studied: infinite gratings, finite gratings, infinite cross-gratings. These are pictorially represented in Fig. 1.

Typically, RCWA simulations show a smooth and continuous variation over a range of physical and valid parameters. Comparing these to experimental data obtained from an ellipsometer, one can fit parameters such as CD, side wall angle, height, etc. In the literature, much has been written about the errors associated with this process and how to maximize precision [13], [14]. Most commonly, the resulting precision will be on the order of angstroms such as in [15]. For a fully optimized system measuring silicon fins, this precision is reduced to about 20 picometers as seen in [16]. The structure we propose achieves precision below 10 picometers without optimization.

The motivation for this work is provided by the semiconductor industry where characterization of thin metal lines is becoming increasingly difficult with demand for small line widths to keep up with Moore’s law. As such, our structure will be designed to be easily integrable into the existing process flow. Since copper is used extensively in the semiconductor fabrication process, that will be the metal of interest even though the noble metals could yield improved results.

2. Background theory

Our simulations will be presented in terms of the Mueller matrix element $M_{12}$. Since we are using an angle of incidence of 65 degrees along the length of the thin grating lines, the sample can be characterized fully by the standard spectroscopic ellipsometry variables $\psi$ and $\delta$ though only one is needed for these initial simulations and we know $M_{12} = -\cos 2\psi$ [17]. Note that if the angle the projection of the incident light makes with the grating is not a multiple of $\pi/2$, the full Mueller matrix is needed to characterize the structure. As expected, the simulations produced only 3 unique nondegenerate values ($M_{12}$, $M_{34}$ and $M_{44}$) validating our stated assumptions. As detailed in [18], plasmons will appear as dips in the spectra for $\psi$ and hence also for $M_{12}$ due to absorption of TM-polarized light for the given conditions. Note that this work uses grating coupling rather than prism coupling for increased flexibility.

At this time, the grating structure used by the semiconductor industry for scatterometry measurement of line width is an infinite grating as shown in Fig. 1(a). It is well known that for metallic gratings, incident light can couple with free electrons to produce plasmons [19]. For the case of a one dimensional grating with a period of 120 nm, no plasmonic activity can be generated as this period is much too small to allow for effective coupling to a surface plasmon and lacks confinement for coupling to a localized plasmon, see Fig. 2. From the graph below, we see minor variation in the spectra but these can only be used to separate structures that have line thickness differences on the order of nanometers. In reality, roughness and local variation in structure would increase the amount of fitting that needs to be done and the overall error, limiting how much useful information can be taken from the spectra. Note that sensitivity for one dimensional metallic gratings does not improve with increasing or decreasing period as compared to Fig. 2.

The main feature in Fig. 2 from 575 to 650 nm arises from the dielectric function of copper. From [20], interband transitions begin to occur at 2.08 eV or 596 nm. Keeping these simulations as the baseline, any variation we see in the next two sections will necessarily be due to geometrical factors and plasmonic excitations. In order to overcome this lack of useful plasmonic coupling in infinite gratings with such small pitch, we designed an infinite cross-grating
structure. The added grating is approximately an order of magnitude larger for both pitch and line width and is thus termed the larger dimension. This structure can be easily modified to shift the CD sensitive region as needed by varying the pitch or line width of either dimension.

3. Simulation setup

As our simulations rely on RCWA, the structures for this paper are all finite in the z-direction and infinitely periodic in the x and y directions. In practice, these conditions will not affect ellipsometric measurement as even small spot areas are a couple of orders of magnitude larger than the structure features [21]. Note that we first confirmed the results from [18] to make sure that our software produced accurate spectra for known, experimentally verified conditions. Taking into consideration the issues with RCWA and metallic cross-gratings as seen in [22], the simulations presented here have been thoroughly checked for convergence.

In this paper, a structure that is sensitive to CD variation will be required to have a difference in $M_{12}$ greater than 0.01 per change in CD. This constraint guarantees that the simulations are significant with respect to systematic errors. For these simulations, we will take the change in CD to be 1 Å in order to demonstrate certain angstrom scale sensitivity.

To make a more experimentally realizable structure, the simulations were performed with the gratings surrounded by a thin TaN barrier layer of 6 Å to prevent Cu diffusion. The TaN coating thickness was determined from [23] while the remaining parameters were varied to optimize sensitivity. Note that cobalt, which is often used experimentally instead of TaN, has also been simulated and does not dampen the plasmonic effects seen. For all simulations presented, the gratings are 50 nm tall and the oxide fill extends 20 nm below the copper with all remaining parameters varied as stated.

4. Results and discussion

4.1. Infinite cross-grating

Looking at the spectra in Fig. 3, the majority of the variation (between 600 and 1200 nm) is due to localized plasmons caused by small changes in the effective refractive index of the structure as seen in [24]. The locations of the minima are presented in Table 1 in the first appendix section.
Fig. 3. Infinite cross-grating, $P_y = 1200$ nm, $L_y = 100$ nm, $P_x = 75$. Main feature due to localized plasmon coupling.

Fig. 4. Each bar represents the window in which a plasmonic resonance is visible in the spectra above 800 nm resulting in CD sensitivity. Infinite cross-grating, $P_y = 875$ nm, $L_y = 100$ nm, $\Delta P_x = 10$ nm, $\Delta CD = 0.5$ nm.

Experimentally, there are often limitations placed on what structures can be produced given the materials and desired design. The most challenging quantities to vary are the smaller dimension line width and period. To ensure that our structure is useful for whatever CD or $P_x$ is produced, simulations were performed that vary both of these quantities over a large range of values. Figure 4 summarizes these simulations and shows two important trends. First, each cross-grating is demonstrating equivalent sensitivity over a certain range of CDs summing to about one-third of the total range. Second, there is a general trend visible based on the fill factor - the ratio of area filled by the grating to the total area [25] - which is expected due to the nature of localized plasmons.

As an example, the ranges centered about $(P_x = 60, CD = 13.5), (70, 16), (80, 19),$ etc. all
have fill factors near 0.315. This also explains the trend of increasing range of sensitive CDs as the fill factor for both lower and upper limits remains approximately equal. For more information on this fill factor connection and variation of the larger dimension pitch, see the appendix. As expected based on the above results, simulations have shown that sensitivity holds for CD changes less than 10 picometers allowing for picometer scale sensitivity when the peaks are fitted appropriately.

4.2. Finite grating

![Finite Grating, CD Variation](image)

Fig. 5. Finite grating, $P_y = 1200$ nm, $L_y = 100$ nm, $P_x = 75$ nm.

At first glance, one might expect this structure to produce spectra more similar to the infinite grating than the infinite cross-grating. Because of the periodic absences in this structure, localized plasmons are produced and the dips associated with them are present. This can be seen in Fig. 5.

Due to the change in refractive index and reduced propagation length compared to the cross-grating, the finite grating spectra is more compact. As indicated in Table 2 in the first appendix, the structure barely retains sensitivity for the given parameters. Compared to the infinite cross-grating, the finite grating is 3 times less sensitive. While angstrom scale sensitivity has been demonstrated, picometer resolution was not obtainable for the finite grating case.

5. Conclusion

We have simulated two experimentally realizable structures and shown how their spectra is extraordinarily sensitive on the critical dimension of extremely thin gratings. The simulated structures have dimensions and materials that are representative of the copper metal lines used in the semiconductor industry. Because of its larger range of sensitivity, the infinite cross-grating is the choice for future fabrication. Note that the added pitch for the cross-grating is large enough so that we will not be limited by lithographic constraints.

Though not presented here, these results have shown resilience to minor variations in roughness, rounding and side wall angle with regards to sensitivity. Additionally, removing the oxide fill and the TaN adhesion coating showed equivalent sensitivity for each case though the spectra
shifts around. More simulations were performed over a wide range of periods and line widths with only the optimal desired results presented.

Additional simulations show that nonmetallic gratings lack any sensitivity or minima compared with metallic gratings. If another CD or periodicity is required, the oxide fill or material composition could be altered to obtain equivalent results. Given this flexibility, we fully expect similar fabricated structures to demonstrate angstrom scale sensitivity to CD variation. Experimental verification is anticipated once samples are produced.

6. Appendix

6.1. Minima values for presented plots

Presented here are the locations of each minima pictured in the plots for CD variation. The first table corresponds to Fig. 3, the second corresponds to Fig. 5.

Table 1. Infinite cross-grating dip location v. CD, bold values indicate structure demonstrates angstrom scale sensitivity as required. The minima shifts up 3.06% of its initial location per 1 Å increase in CD on average with a standard deviation of 1.06 nm.

<table>
<thead>
<tr>
<th>CD</th>
<th>16.5</th>
<th>16.6</th>
<th>16.7</th>
<th>16.8</th>
<th>16.9</th>
<th>17.0</th>
<th>17.1</th>
<th>17.2</th>
<th>17.3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dip location</td>
<td>879</td>
<td>890</td>
<td>923</td>
<td>945</td>
<td>967</td>
<td>1000</td>
<td>1021</td>
<td>1054</td>
<td>1098</td>
</tr>
</tbody>
</table>

Table 2. Finite grating dip location v. CD, bold values indicate structure demonstrates angstrom scale sensitivity as required. The minima shifts up 1.06% of its initial location per 1 Å increase in CD on average with a standard deviation of 0.31 nm.

<table>
<thead>
<tr>
<th>CD</th>
<th>16.5</th>
<th>16.6</th>
<th>16.7</th>
<th>16.8</th>
<th>16.9</th>
<th>17.0</th>
<th>17.1</th>
<th>17.2</th>
<th>17.3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dip location</td>
<td>976</td>
<td>982</td>
<td>994</td>
<td>1001</td>
<td>1014</td>
<td>1026</td>
<td>1037</td>
<td>1045</td>
<td>1057</td>
</tr>
</tbody>
</table>

6.2. Experimental considerations

As stated above, the enhanced sensitivity seen in the cross-grating structure is seen even when side wall angle and rounding variations are considered. Due to the link between side wall
angle and CD, this result is unsurprising. As for rounding variation, even lines with completely rounded tops demonstrate enhanced sensitivity as seen in Fig. 6.

Regarding defect analysis, these structures will be extremely sensitive to large scale or periodic defects. Characterization of such defects would be routine for RCWA and may lead to a better understanding of their cause. Considering the spot size of the ellipsometer and the feature dimensions of this structure, a few small defects would be hard to detect and would only marginally affect the output.

6.3. Fill factor

As a demonstration of the importance of fill factor with respect to the sensitivity of the cross-grating structure, we present Fig. 7 simulating 6 structures of approximately equal fill factor. The smaller number in the legend represents the CD and the larger number represents the smaller dimension period. This shows that within a few nanometers of CD and tens of nanometers in smaller dimension period, fill factor is the key parameter for characterization. Though some differences between the spectra are visible, they would not in practice be easily separable with just $M_{12}$ plots.

Acknowledgments

Thanks to Nanometrics for funding and use of their Nanodiffract software which was used for all RCWA simulations. The schematics of the gratings were produced using SketchUp Make.