Robust profile reconstruction in optical scatterometry

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Recently, optical scatterometry has been introduced to monitor the critical dimension and overlay of grating structures in semiconductor manufacturing [1]. As a model-based technique, its success heavily relies on the effectiveness of profile reconstruction, which is usually formulated as a nonlinear least squares inverse problem in the form of

$$\hat{\mathbf{x}} = \arg\min \left\{ [\mathbf{y} - \mathbf{f}(\mathbf{x})]^{\mathrm{T}} \mathbf{W} [\mathbf{y} - \mathbf{f}(\mathbf{x})] \right\}, \tag{1}$$

where **y**, **f**(**x**), **W**, and **x** represent the measured signature, the forward operator, the weighting matrix, and the profile parameters that characterize the grating structure, respectively.

In general, any gradient-based method such as Gauss-Newton iteration (GNI) algorithm can be used to obtain an optimal solution $\hat{\mathbf{x}}$. This is done by using the Taylor expansion and by linearizing the cost function $[\mathbf{y} - \mathbf{f}(\mathbf{x})]^{\mathrm{T}} \mathbf{W} [\mathbf{y} - \mathbf{f}(\mathbf{x})]$ in a small domain of **x**, which leads to the form

$$\Delta\mathbf{x} \approx -[\mathbf{J}(\mathbf{x})^{\mathrm{T}} \mathbf{W} \mathbf{J}(\mathbf{x})]^{-1} \mathbf{J}(\mathbf{x})^{\mathrm{T}} \mathbf{W} \Delta\mathbf{y}, \tag{2}$$

where **J**(**x**), Δ**x** and Δ**y** are the Jocobian, the parameter departure, and the signature residual between the measured and calculated signatures, respectively.

Equation (2) is repeatedly calculated in the GNI algorithm until convergence to an optimal solution $\hat{\mathbf{x}}$ is reached. As shown in Eq. (2), it is obvious that the accuracy of Δ**x** is directly related to the signature residual Δ**y**. Consequently, by directly using Eq. (2), Δ**x** will be badly influenced by Δ**y** if there exist any outliers in the measured signature **y**.

In this paper, we report a method to eliminate the bad effect of outliers in Δ**y** on Δ**x** at each iteration by introducing the principle of robust estimation [2]. The key point of our method is to reformulate Eq. (2) as $\Delta\mathbf{y}^{\mathrm{T}} \approx \Delta\mathbf{x}^{\mathrm{T}} [-\mathbf{J}(\mathbf{x})]^{\mathrm{T}}$ with a Moore-Penrose pseudoinverse and then to iteratively minimize

$$\left\{ \Delta\mathbf{y}^{\mathrm{T}} - \Delta\mathbf{x}^{\mathrm{T}} [-\mathbf{J}(\mathbf{x})]^{\mathrm{T}} \right\}^{\mathrm{T}} \mathbf{W}_{\mathrm{L}}(\Delta\mathbf{x}^{\mathrm{T}}) \left\{ \Delta\mathbf{y}^{\mathrm{T}} - \Delta\mathbf{x}^{\mathrm{T}} [-\mathbf{J}(\mathbf{x})]^{\mathrm{T}} \right\}, \tag{3}$$

where $\mathbf{W}_{\mathrm{L}}(\Delta\mathbf{x}^{\mathrm{T}})$ is another weighting matrix as a function of $\Delta\mathbf{x}^{\mathrm{T}}$. Note that the only unknown parameter in Eq. (3) is Δ**x**, as **J**(**x**) can be calculated in advance.

Figure 1 depicts the cross-section SEM image of an investigated silicon grating with profile parameters of *TCD*, *Hgt*, and *BCD*. Figures 2 and 3 present the reconstructed profile parameters via simulation and experiment by using the GNI and our proposed method. These results have demonstrated that our proposed method outperformed the conventional GNI algorithm.

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[1] C. J. Raymond, M. R. Murnane1, S. L. Prins, S. Sohail, H. Naqvi, J. R. McNeil, and J. W. Hosch, J. Vac. Sci. Technol. B **15**, 361 (1997)

[2] P. J. Huber and E. M. Ronchetti, *Robust Statistics* (John Wiley & Sons, New York, 2009).

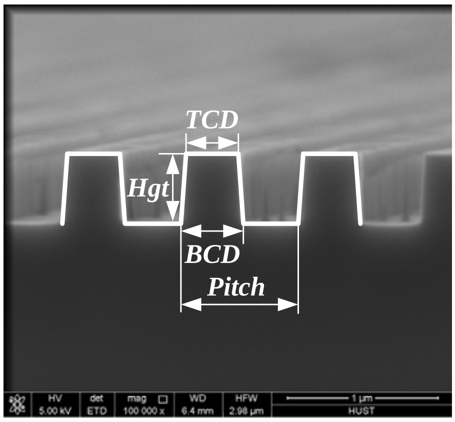

Figure 1: The cross-section SEM image of the investigated one-dimensional trapezoidal silicon grating.

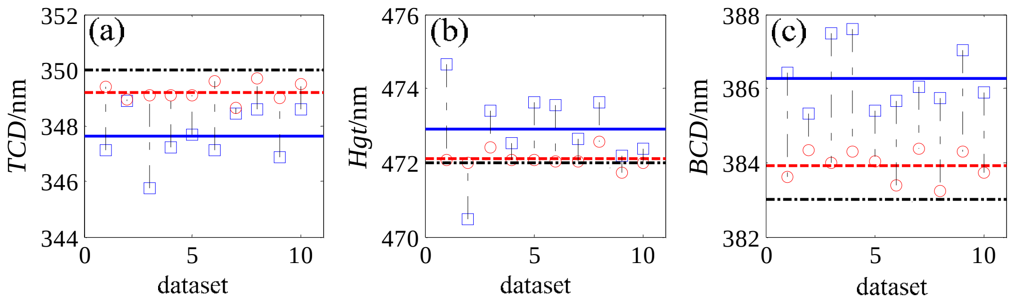

Figure 2: The simulated reconstructed values of (a) TCD, (b) Hgt and (c) BCD for ten simulated tests by using the GNI algorithm and our proposed method. Blue squares and blue lines represent the reconstructed values and their mean by the GNI algorithm respectively. Red circles and red dotted lines represent the reconstructed values and their mean by our proposed method respectively. Black dashed lines represent the actual values.

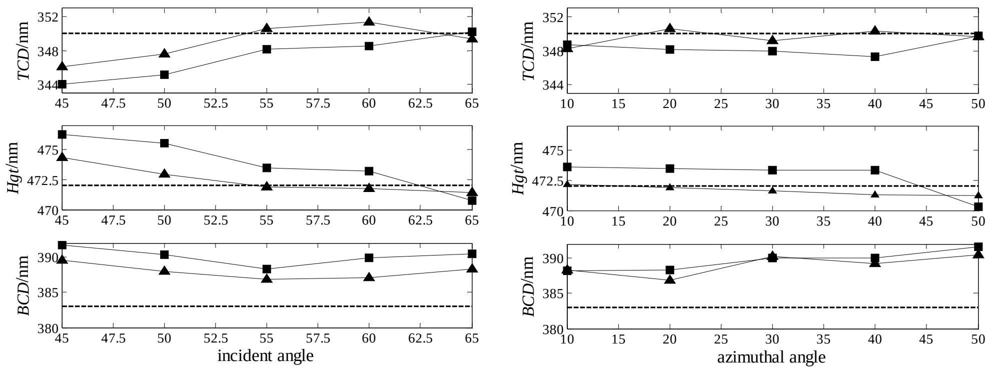

Figure 3: The experimental reconstructed values of TCD, Hgt and BCD using the GNI algorithm and our proposed method under the varying (a) incident angle and (b) azimuthal angle. Black squares and triangles represent the reconstructed values obtained by the GNI algorithm and our proposed method respectively. Black dotted lines represent the SEM measured values.