Computational metrology for nanomanufacturing

Shiyuan Liu [a, b, *]

[a] Wuhan National Laboratory for Optoelectronics, Huazhong University of Science and Technology, Wuhan 430074, China;

[b] State Key Laboratory of Digital Manufacturing Equipment and Technology, Huazhong University of Science and Technology, Wuhan 430074, China

ABSTRACT

One critical challenge for high-volume nanomanufacturing requires the on-line monitoring and measurement of the nanostructures manufactured. Computational metrology is expected to provide a novel means for fast, low-cost, non-destructive, and accurate measurement in high-volume manufacturing. Computational metrology refers to a measurement method where a complicated measurement process is modeled as a forward problem and some measured data are obtained by a specific instrument under a certain measurement configuration, and then the measurands are precisely and accurately reconstructed by solving the corresponding inverse problem. Thus computational metrology is essentially a model-based metrology and a typical process to solve an inverse problem. The key issues in computational metrology, such as the measurability, the measurement error analysis and precision estimation, the measurement configuration optimization, the fast and accurate forward modeling, and the fast and robust measurand reconstruction, and their generalized solution methods are explored in this paper, with an emphasis on the significance and necessity to apply modern mathematical theories and tools in solving the related problems. Some case studies carried out in my research group are presented to demonstrate the capability of computational metrology.

Keywords: computational metrology, model-based metrology, measurability, measurement error analysis, measurement configuration, model order reduction, inverse problem solving.

1. INTRODUCTION

Nanomanufacturing refers to the manufacturing of products with feature dimensions at the nanometer scale. It is an essential bridge between the newest discoveries of fundamental nanoscience and real-world products by nanotechnology. For nanotechnology-enabled products to achieve broad impacts to society and to promise huge benefits to our everyday lives, they must be manufactured in market-appropriate quantities by reliable, repeatable, economical, and commercially viable methods [1].

One critical challenge to the realization of nanomanufacturing is the development of necessary instrumentation and metrology at the nano-scale, especially the fast, low-cost, and non-destructive measurement methods that are suitable in high-volume nanomanufacturing [2,3]. For instance, in dimensional measurement, coordinate measuring machines (CMM) are commonly used at the macro-scale, and vision-based optical methods are well suitable at the micro-scale; nevertheless, when the dimension further goes down to the nano-scale, the vision-based optical metrology seems to be helpless [4,5]. The currently available metrology tools such as scanning electron microscope (SEM), transmission electron microscope (TEM), atomic force microscope (AFM), and scanning probing microscope (SPM), are capable of meeting the exploratory nano-scale research, but are of disadvantages in their low speed, high cost and the difficulties to be integrated into the manufacturing process [6,7].

In recent years, model-based metrology has made a new path to the on-line and nondestructive measurement in high-volume nanomanufacturing [8,9]. By utilizing the interactions between the measurands and the physical fields such as the electromagnetic scattering field, the acoustic scattering field, and the temperature field, the model-based metrology solves an inverse problem to reconstruct the related information from the measured data that are obtained by some

* Corresponding author: shyliu@mail.hust.edu.cn; phone: +86 27 8755 9543; webpage: http://www2.hust.edu.cn/nom.

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instruments. The principle of such a measurement method is the interaction mechanism between the physical field and the measurands, which is usually described by some complicated partial differential equations such as Maxwell equations. Hence, there are two key points of this kind of metrology, one is the forward modeling to establish a complicated nonlinear model with multiple input and output parameters, the other is the inverse problem solving to accurately and precisely reconstruct the measurands from the measured data by using some iterative optimization algorithms.

The model-based metrology has been studied for years, and some results have been achieved on the forward modeling and inverse problem solving. But in general, most of the research work focuses on specific applications, and the methods proposed do not have sufficient generality and universality. As the model-based metrology involves vast complicated scientific computational problems, I recently termed it as "computational metrology" [10]. In this paper, I will introduce the fundamental concepts of computational metrology, explore the key issues involved in computational metrology, and discuss their generalized solution methods. I will also present some case studies carried out in my research group to demonstrate the capability of computational metrology.

2. FUNDAMENTAL CONCEPTS

Metrology is defined by the International Bureau of Weights and Measures (BIPM) as "the science of measurement, embracing both experimental and theoretical determinations at any level of uncertainty in any field of science and technology" [11]. Metrology consists of the investigation on new principles of measurement as well as applications of new mathematical methods of data analysis. Thus, except for the improvement of the metrology instruments, the progress of metrology also heavily relies on the development of new mathematical tools and their applications.

In a practical application of metrology, the measured data are obtained by a measurement system (i.e. instrument) utilizing some physical or chemical sensing principle, and the measurands can be reconstructed by further data analysis. If the measurands and the measured data are treated as the input and output of the measurement system, respectively, an abstract mathematical model that relates the input and output is necessary to describe and analyze the static and dynamic properties of the measurement system. Therefore, a complete measurement system consists of both of the measurement system and the corresponding mathematical model.

For an ideal measurement system, the mathematical model is simply a linear transfer function, which relates the output (measured data) to the input (measurands) with the most convenience for measured data analysis. For a practical measurement system, the mathematical model is usually nonlinear due to the existence of unavoidable distortion and drifting, and the measurement system may be abstracted as a weakly nonlinear transfer function with noise. In order to directly reconstruct the measurands from the measured data in such a system, some mathematical compensation algorithms were usually designed for the system linearization. For instance, when measuring the displacement by using a capacitive sensor with its polar distance varying, the measured data are the variations of capacitance between the polar plates, and the measurands are the variations of the polar distances. Although the relationship between the capacitance and distance changes is nonlinear, the capacitance variation can be approximately regarded as a linear function of the displacement variation if the distance variations are restricted in a small region. Then the displacement variation can be directly obtained by measuring the capacitance variation.

However, for some measurement systems with multiple input and multiple output parameters, the transfer function between the input and output has to be described by a very complicated nonlinear mathematical model. For such a measurement system, the measurands cannot be obtained from the measured data in an explicit form. Instead, the measurands can only be reconstructed by solving an inverse problem, which involves complicated physical and mathematical modeling and inverse problem solving. For instance, recently optical scatterometry has been demonstrated as one of the most promising candidates for fast, noncontact, nondestructive, and of low-cost metrology of nanostructures [12]. The input of optical scatterometry includes the measurands such as the critical dimension (CD), height, and sidewall angle (SWA) of the nanostructure, and the measurement configuration such as the wavelength, the incident angle, and the azimuthal angle, while the output is the scattered spectrum such as in the form of reflectivity, ellipsometric angles, Stokes vector elements, or Mueller matrix elements. As the transfer function relating the input to the output is too complicated and nonlinear, it is too difficult to directly obtain the measurands from the measured data. In order to reconstruct the measurands, it requires to establish a forward model such as Maxwell equations to relate the output to the input, followed by calculating the model by using methods such as rigorous coupled-wave analysis (RCWA) and thin film transmission theory [13], as shown in Figure 1. Then, the measurands such as the nanostructure CD are reconstructed from the measured data by solving the corresponding inverse problem with the objective to find an optimal input whose calculated output can best match the measured data by using some iterative optimization algorithms [14-16].

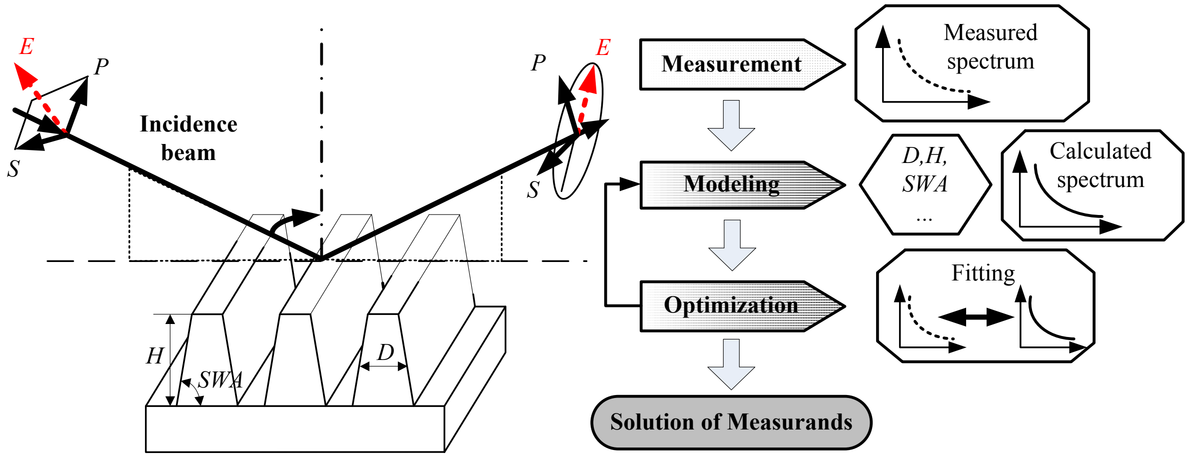

Figure 1. Principle of optical scatterometry.

As the metrology process of such nonlinear measurement systems involves vast and complicated scientific computations, especially numerical computations, I recently termed such kind of model-based metrology as "computational metrology" [10]. Here, I further define it as "a measurement method where a complicated measurement process is modeled as a forward problem and some measured data are obtained by a specific instrument under a certain measurement configuration, and then the measurands are precisely and accurately reconstructed by solving the corresponding inverse problem." I summarize the fundamental principles of computational metrology, whose basic elements include the measurands, measurement configuration, forward model, measured data, and solution of measurands, as shown in Fig.2. I also emphasize that computational metrology should include at least three fundamental characteristics as follows:

(1) Computational metrology is essentially a model-based metrology, whose measurement system requires a complicated forward transfer model with multiple input and output parameters.

(2) Computational metrology is typically an inverse problem solving process, and its success heavily relies on two key techniques. One is the forward transfer modeling and its fast algorithm, and the other is the inverse problem solving and its robust algorithm.

(3) The objective of computational metrology is quantitative measurement. The final solution of the measurands should and could be quantitatively evaluated by measurement error, accuracy, precision, and/or uncertainty. It is essentially different from the problems such as the model-based fault-diagnosis where only the judgment of fault existence is required.

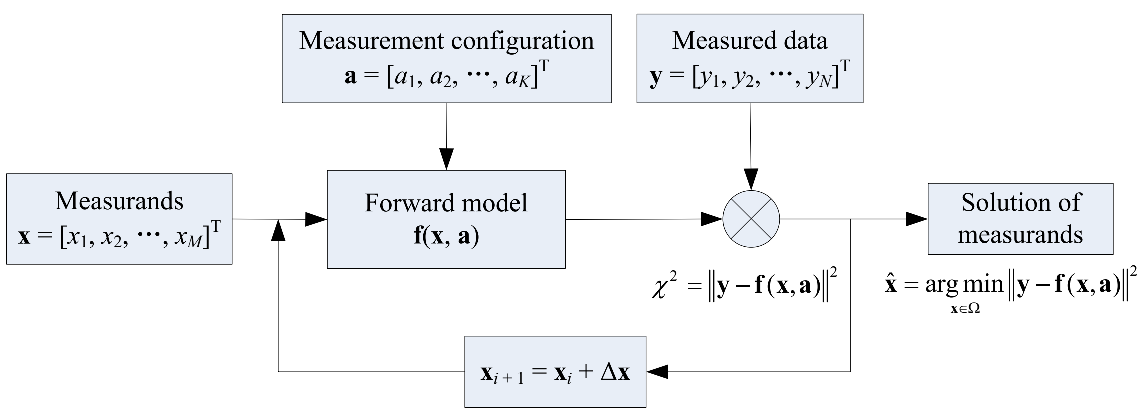

Figure 2. Fundamental concepts and basic elements of computational metrology.

3. KEY ISSUES

Based on the characteristics of computational metrology, I summarize the following key issues in computational metrology.

3.1 Measurability

Essentially, computational metrology is a kind of metrology to obtain the measurands from the measured data by solving an inverse problem related to a complicated physical model. Here, a fundamental question should be answered first: In what condition the true value of the measurands can be obtained accurately and precisely? We call it the problem of measurability in computational metrology. It is the theoretical foundation for us to select a measurement method, to establish a measurement system, and to analyze the measured data in computational metrology. Most of the existing work pays more attention to the techniques of the forward modeling and the inverse problem solving, and the rigorous explanation and demonstration of measurability is neglected. In fact, many solution methods to inverse problems did not have rigorous proofs until 1980. After 1980, it turned to be an active area with a solid theoretical foundation, and some important theoretical problems were solved, such as the existence and uniqueness of solutions to inverse problems [17-20]. However, many simplifications and ideal assumptions were made to solve these problems, and these assumptions cannot be satisfied or fully satisfied in the practical engineering applications. For example, the real measurement systems are only capable of obtaining a finite number of data at finite points in the physical field. Therefore, the measurement information is limited, leading to the solution to the corresponding inverse problem being ill-posed.

3.2 Measurement error analysis and uncertainty evaluation

As the objective of computational metrology is to quantitatively determine the value of the measurands, the measurement error analysis and uncertainty evaluation is another important foundational problem. Currently, the error analysis theory has become very mature, and has been comprehensively employed in conventional measurement systems to analyze the measured data with errors [21]. However, the errors in computational metrology are not only from the measured data, but also from the forward model adopted. These errors will be transferred to the final solution of the measurands. Most of the existing work focuses on how to solve the inverse problem and only present the solution alone. The uncertainty of the solution is usually ignored [22,23]. It may be acceptable for other inverse problems, but for computational metrology that requires precise and accurate measurement, the solution as well as the estimation of its uncertainty are both necessary. Hence, further studies are needed to address these issues, including the source and property of errors, the mechanism of error propagation during solving the inverse problem, and the evaluation of measurement uncertainty.

3.3 Confliction of measurement speed and accuracy

The objects of modeling in computational metrology are usually the complicated physical fields, such as electromagnetic field, acoustical field, pressure field, and temperature field. These physical fields can be described by using a series of non-linear partial differential equations, such as Maxwell equations, Helmholtz equations, Poisson equations, and Laplace equations [24]. Numerical method, such as finite element method, finite volume method, finite difference method, and boundary element method [25], is usually the only way to solve such complicated nonlinear partial differential equations. Generally, a higher accuracy can be achieved by refining a smaller mesh/grid, but with the penalty of more runtime. Although numerous skillful algorithms with powerful hardware have been introduced and developed, it is still difficult to satisfy both the speed and accuracy demands of the complicated modeling and simulation. In addition, among the iterative optimization algorithms used to solve the inverse problems, the stochastic optimization algorithms usually guarantees a global optimal solution but its time cost is too expensive, while the deterministic optimization algorithms converge relatively fast but a global optimal solution is usually not guaranteed.

4. SOLUTION METHODS

By exploring the key issues in computational metrology, it is noted that solving these issues relies on the modern mathematical theories and tools, including integral-differential equations, functional analysis, Hilbert space, distribution theory, variational method, probability theory and statistics, matrix theory, numerical implementation, inverse problem, and optimization method. By combining these mathematical theories and tools with metrology science, computational electromagnetism, and computational acoustics, it is expected to develop a general set of solution methods for computational metrology.

4.1 Measurability

The measurability of computational metrology can be studied by applying the functional analysis, especially the mathematical theory for inverse problems. Similar to many other inverse problems, computational metrology can be expressed as a nonlinear operator equation such as y=Ax, where A: X->Y represents the nonlinear operator that characterizes the input/output transfer function of the measurement system, and X and Y are Hilbert spaces. The measurability of computational metrology can be mathematically defined as: Under the condition of a given operator A and measured data y, whether there is a solution for the measurands x, whether the solution is unique, and whether the solution is stable (i.e, whether the measurands x continuously depend on the measured data y)? As long as one of these three basic conditions is not satisfied, the related inverse problem is called ill-posed [20]. From this point of view, the problem of computational metrology under the condition of a given physical model and finite measured data is usually ill-posed. In practical engineering applications, the measured data are usually discrete and inevitably include various kinds of noise. The nonlinear operator that characterizes the input/output transfer function of the system also contains errors such as model simplification error and numerical calculation error. All these facts could further intensify the ill-posed problem in computational metrology. In order to achieve the measurability of computational metrology, we need to introduce apriori information to limit the solution space. From the viewpoint of functional analysis, it is equivalent to build a compact set K ($K \subseteq X$) in the Hilbert space X where the solution is included. At the same time, Tikhonov regularization methods can be introduced to convert and redefine the computational metrology problem to a functional minimization problem, which approximates the solution of the equation y=Ax by using the minimum value x^* of this function. Therefore, the measurability of computational metrology is changed to be the problem of existence, convergence, and stability of the minimum of this function. Denote this function as T(x), which contains two parts: one is called the cost function that evaluates the distance from the true value to x^*, and the other is called the regularization term that represents the smoothness limit of the solution and all the apriori information. By analyzing if the function $T(x)$ is closed, bounded, dense, and monotone, we may judge if its solution is existent, unique, and numerically stable, and this judgment answers the measurability question of computational metrology [26].

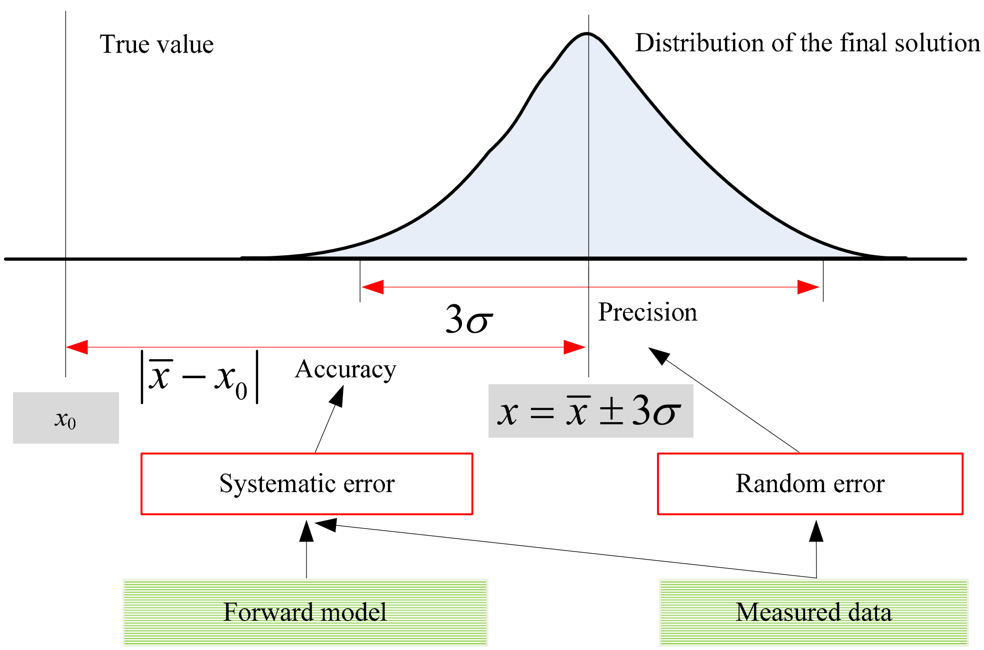

Figure 3. Error source and its effect on the final solution of measurands in computational metrology.

4.2 Error analysis and uncertainty evaluation

Figure 3 shows the source of errors and their influence on the final solution of measurands in computational metrology. The random error, usually induced by the random noise of the measured data, mainly affects the precision of the solution. The systematic error mainly affects the accuracy of the solution, which is usually induced by two aspects of factors: the measurement system (instrument) and the forward model. The random error can be treated as a random variable, which can be estimated based on probability and mathematical statistics. The covariance matrix of the measurands can be obtained by calculating their Hessian matrix with the measured data, resulting in the variance of each measurand and the correlation coefficients between different measurands. With this information, we may further evaluate the precision of the measurands and their coupling effects. As for the systematic error, we may apply a first-order Taylor expansion for the cost function that is formulated for the inverse problem. This Taylor expansion is usually performed near the solution of the measurands and under the nominal measurement configuration, leading to an error propagation matrix whose elements can be used to evaluate the influence of the systematic error on the measurement accuracy of the final solution. All these error analysis methods may be further used to reduce the measurement error and to improve the measurement precision and accuracy.

4.3 Measurement configuration optimization

Measurement configuration refers to a combination of measurement conditions, and the objective of configuration optimization in computational metrology is to balance the tradeoff between the measurement speed and accuracy. First, we need to find an optimal configuration of the measurement system to guarantee the highest sensitivity of the measured data to the measurands. As shown in Figure 4, the measurement system in computational metrology is characterized as a forward model with multiple input and output parameters, a useful tool for configuration optimization is sensitivity analysis on this forward model [27], with the objective to find an optimal measurement configuration with the highest sensitivity. Local sensitivity analysis (LSA) and global sensitivity analysis (GSA) can be used to calculate and analyze the sensitivity coefficients under different measurement configurations [28,29], from which the optimal measurement configuration can be obtained. Then, we may further reduce the measured data as it may contain redundant or even contradictory information for inverse problem solving. Data reduction is to make the size of the measured data as small as possible, but it should be based on the measurability theory to guarantee the existence and uniqueness of the solution.

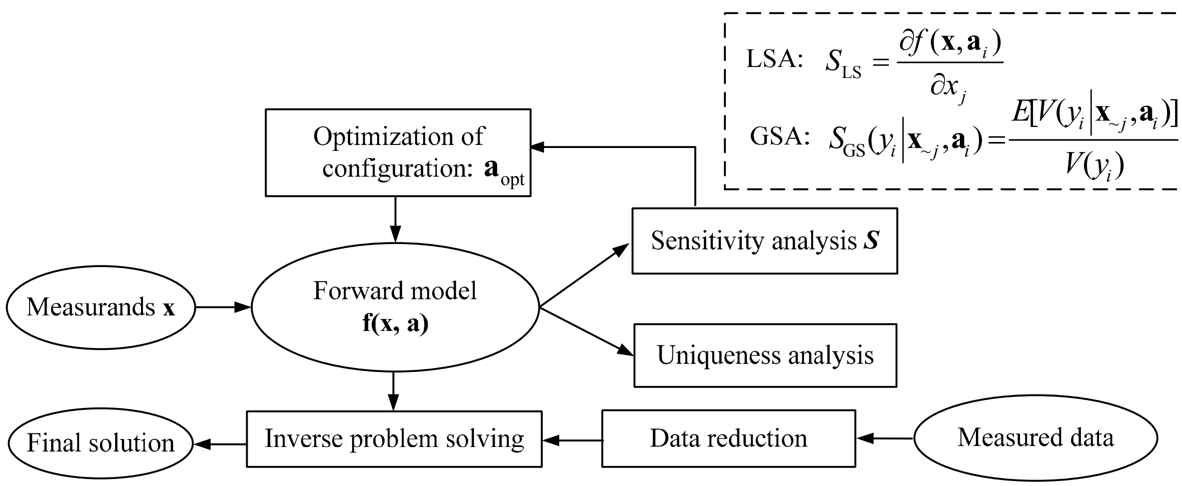

Figure 4. Optimization of measurement configuration in computational metrology.

4.4 Fast and accurate numerical methods for forward modeling

To simulate the complicated physical fields rapidly and accurately, model order reduction (MOR) [30,31] and sparse matrix splitting based coupled-mode (SMS-CM) [32] methods can be introduced into the numerical algorithm of the forward modeling. The MOR method utilizes a reduced data set to construct a lower dimensional Lagrange primary space and to approximate the solution space of the original problem, and then a self-imitation decomposition can be further applied to break the redefined partial differential equations into the measurands-related and unrelated parts. Since the unrelated part can be calculated off-line and the related part only needs some simple algebraic operations, the calculation speed of the model can be improved significantly. To evaluate the accuracy of the solution after MOR, the functional analysis (such as Riesz representation theorem, Babuska-Brezzi conditions, and the dual space) can be used as the theoretical basis to derive and obtain the expression of the error estimation by using the posteriori error estimation method, and the corresponding Lagrange primary function selection algorithm can be further developed. The SMS-CM method expands the physical distribution to be solved by using fixed harmonic basis functions so that a large amount of eigen-problems in the conventional modeling methods (such as the RCWA) may be avoided [13]. As for the dense matrix operation involved in the boundary value problems, the sparse matrix splitting of semi-group can be used to transform the operation of a dense matrix into a sparse matrix. The matrix partition method combined with the fast Fourier transform algorithm can efficiently calculate the products of matrix and vectors, which may dramatically improve the calculation speed.

4.5 Fast and robust measurand reconstruction algorithms

Reconstructing the measurands from the measured data in computational metrology is typically an inverse problem solving process. As described above, in order to ensure the measurability, the ill-posed inverse problem in computational metrology is usually converted to a well-posed optimization problem, which may be solved by some iterative optimization algorithms. One of the key issues is to balance the tradeoff between the algorithm speed and accuracy, particularly when the uncertainty of the measured data is taken into account. At present, the iterative optimization methods can be roughly categorized into two types: the stochastic method [33, 34] and the deterministic method [35,36]. The stochastic method applies random numbers to generate random solutions, and their corresponding probabilities are obtained to guide the search direction. This strategy usually guarantees a globally optimal solution, but with a penalty of high computational cost, particularly when the order of the inverse problem increases. The deterministic method is to approach the optimal solution step by step based on the search direction and step size at each iteration, and the next search is determined from the current location by using its neighboring characteristics (such as its local gradient information). The effectiveness of the deterministic method heavily depends on a good initial guess of the solution. If the initial guess is not suitable, the optimization result is likely to be locally optimal. Therefore, a hybrid optimization algorithm by taking advantage of the effectiveness of the deterministic method and the robustness of the stochastic method may have the potential to balance the tradeoff between the speed and accuracy requirements in computational metrology.

5. CASE STUDIES

Our first example to demonstrate the capability of computational metrology is model-based infrared reflectometry (MBIR) [37-39]. As a particular form of optical scatterometry, MBIR is an attractive optical metrology that has been introduced recently for measuring high aspect-ratio periodic trench structures. As shown in Figure 5, MBIR involves both forward modeling of sub-wavelength trench structures and reconstruction of the measurands from the measured data. In this context, the measurands are the geometric parameters of the trench structure including width and depth, while the measured data contain the scattered optical signatures from the structure in the form of reflectivity spectrum.

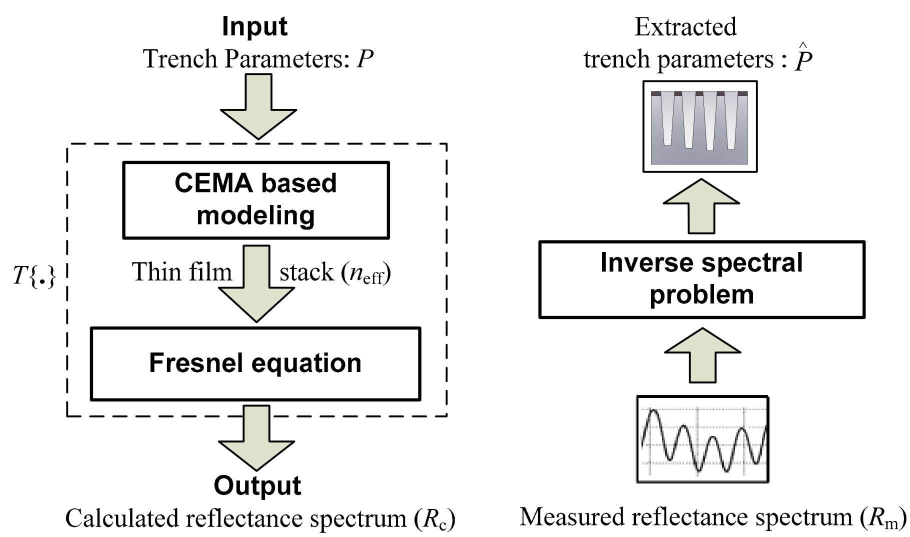

Figure 5. Forward modeling and inverse problem solving in model-based infrared reflectrometry.

MBIR is typically a computational metrology with the objective to find a set of geometric parameters whose calculated reflectivity spectrum can best match the measured ones by using some iterative optimization algorithms. The inverse problem in MBIR is formulated as

$$\hat{P} = \arg\min_P \sum_{j=1}^{N} [R_{\mathrm{m}}(\lambda_j) - T\{P\}]^2 = \arg\min_P \sum_{j=1}^{N} [R_{\mathrm{m}}(\lambda_j) - R_{\mathrm{c}}(\lambda_j)]^2 \quad (1)$$

where $\hat{P}$ represents the optimized solution of the measurands containing a set of geometric parameters; $P=[d_1, d_2, \ldots, d_K, h_1, h_2, \ldots, h_K]$ represents the vector containing geometric parameters of the deep trench structure; d_k and h_k ($k=1,2,\ldots K$) represent the trench width and trench depth of the kth effective layer, respectively; K is the total number of the effective layers; $R_{\mathrm{m}}(\lambda_j)$ and $R_{\mathrm{c}}(\lambda_j)$ represent the measured reflectivity and the theoretically calculated reflectivity, respectively; λ_j represents the jth utilized wavelength and N represents the total number of the utilized wavelengths; $T\{\cdot\}$ represents the forward modeling function transforming the geometric parameter vector P into the theoretically calculated reflectivity $R_{\mathrm{c}}(\lambda_j)$.

In order to achieve fast and accurate forward modeling, we proposed a fast algorithm called corrected effective medium approximation (CEMA) for reflectivity calculation of micro/nano scale high-aspect-ratio deep trench structures [37,38]. The CEMA method is based on the conventional EMA but a dispersion corrected factor is added to calculate the refractive index of each effective medium. The CEMA has been demonstrated to be not only accurate enough but also ten times faster in comparison with the RCWA method. We also developed a method combining the artificial neural network (ANN) and Levenberg–Marquardt (LM) algorithm [39] for robust and fast reconstruction of the geometric parameters from the measured reflectance spectrum, as shown in Figure 6. In the process of parameter reconstruction with the ANN/LM combined method, an initial estimate of the trench parameters is quickly generated from the measured reflectance spectrum by the ANN, and then the accurate solution is obtained by the LM algorithm. The trained ANN alone can only generate a rough estimate of the parameters, which however as an initialization can guarantee the LM algorithm to rapidly converge to an accurate and global solution. The combined extraction method is thus demonstrated to achieve improved performance over the ANN or LM method alone and leads to highly accurate measurement results as well as fast computation speed.

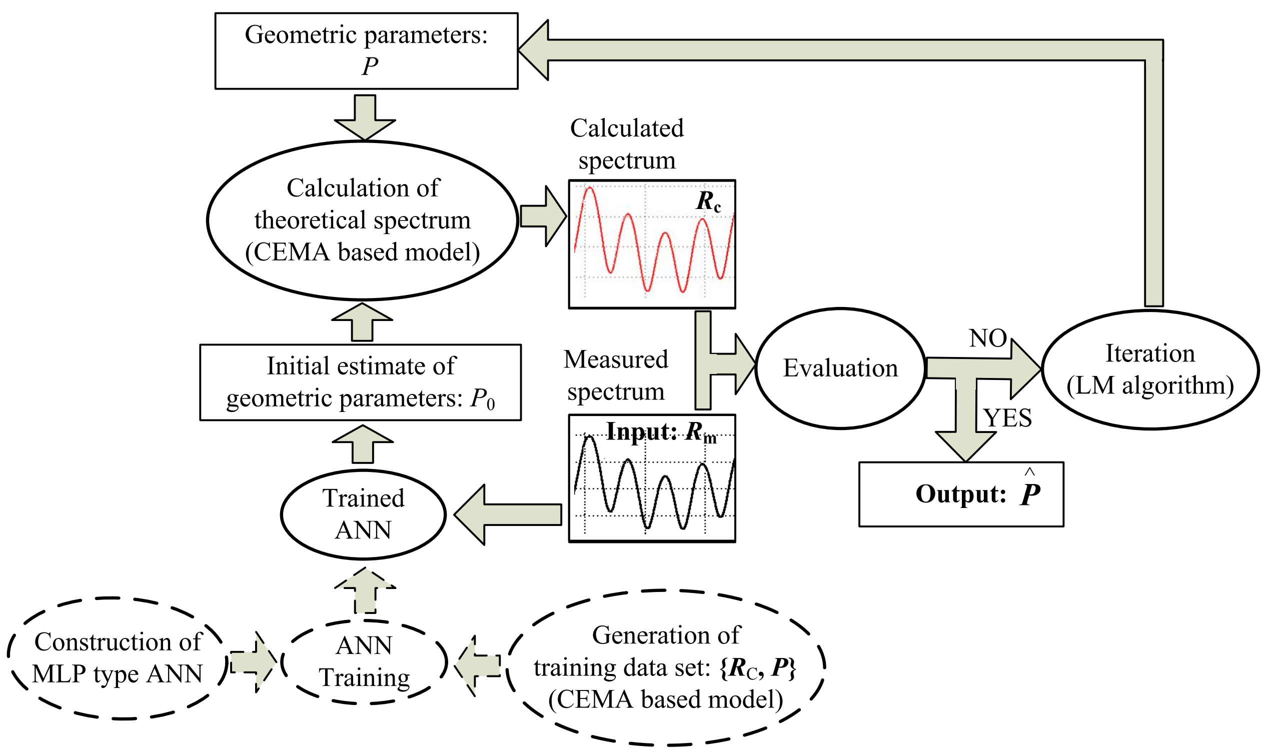

Figure 6. Flowchart of parameter reconstruction using the ANN/LM combined method.

We have set up an experimental platform for MBIR as shown in Figure 7, and have successfully applied the MBIR technique in measuring a bottle trench structure, which is etched on the silicon substrate and filled with polysilicon as electrodes. As shown in Figure 8, this bottle trench structure is a typical design in advanced dynamic random access memory (DRAM) capacitors characterized by four geometric parameters: width of neck layer d_1, depth of neck layer h_1, width of bottle layer d_2, and depth of bottle layer h_2. Figure 8 also depicts the fitted reflectance spectrum calculated from the extracted parameters compared to the measured reflectance spectrum.

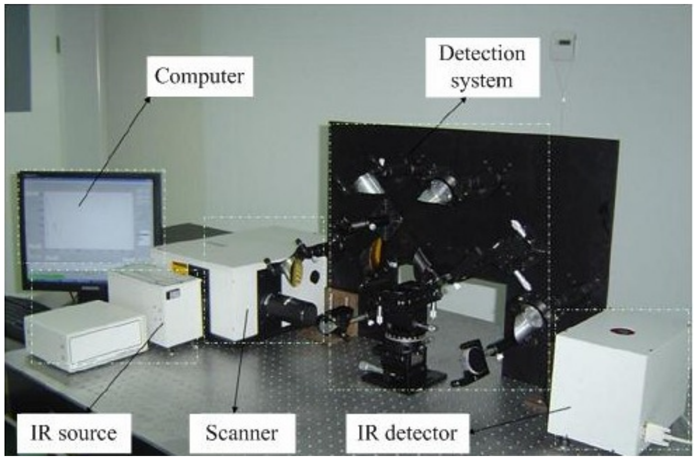

Figure 7. Experimental platform of model-based infrared reflectrometry.

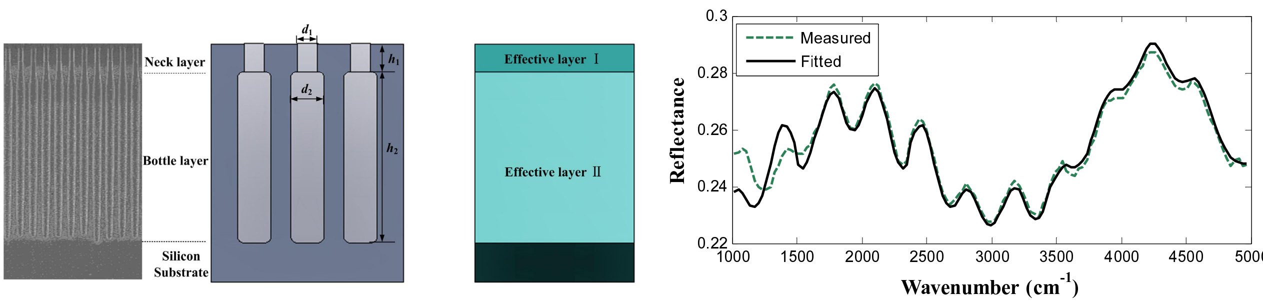

Figure 8. Fitted reflectance spectra calculated from the extracted parameters compared with the measured reflectance spectrum of the bottle trench structure.

Our second example to demonstrate the potential of computational metrology is optical scatterometry based on Mueller matrix polarimetry (MMP) [40-44]. We have developed an MMP prototype suitable from ultraviolet to infrared spectral bands, as shown in Figure 9.. In contrast to the conventional spectroscopic ellipsometry (SE), the MMP can obtain up to 16 parameters of the 4×4 Mueller matrix during each measurement. Consequently, the MMP can obtain much more useful information about the sample than the conventional SE, and thus has potential capability for the metrology of line edge roughness (LER) and line width roughness (LWR) in nanomanufacturing.

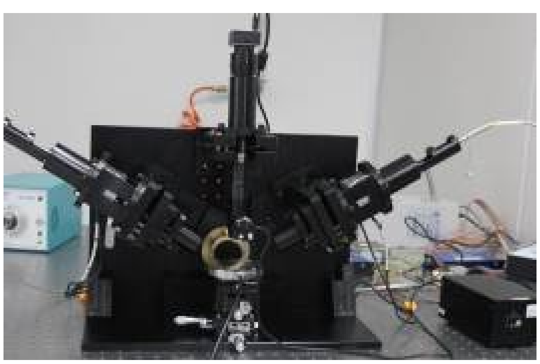

Figure 9. Prototype of Mueller matrix polarimetry.

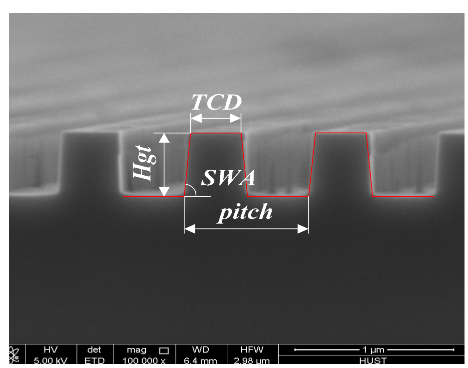

Figure 10. SEM image of silicon grating.

Figure 10 shows a silicon grating structure fabricated by nanoimprint lithography (NIL) process, and Table 1 depicts the reconstructed geometric parameters by MMP compared to those measured by SEM. As can be observed from Figure 11, there is an excellent agreement between the measured and best fitted Mueller matrices.

Table 1. Reconstructed geometric parameters by MMP compared to those measured by SEM

Geometric parameters	**MMP**	**SEM**
Top CD (TCD)	355.14 ± 0.18 nm	350 nm
Height (Hgt)	467.68 ± 0.17 nm	472 nm
Sidewall Angel (SWA)	87.95 ± 0.02°	88°

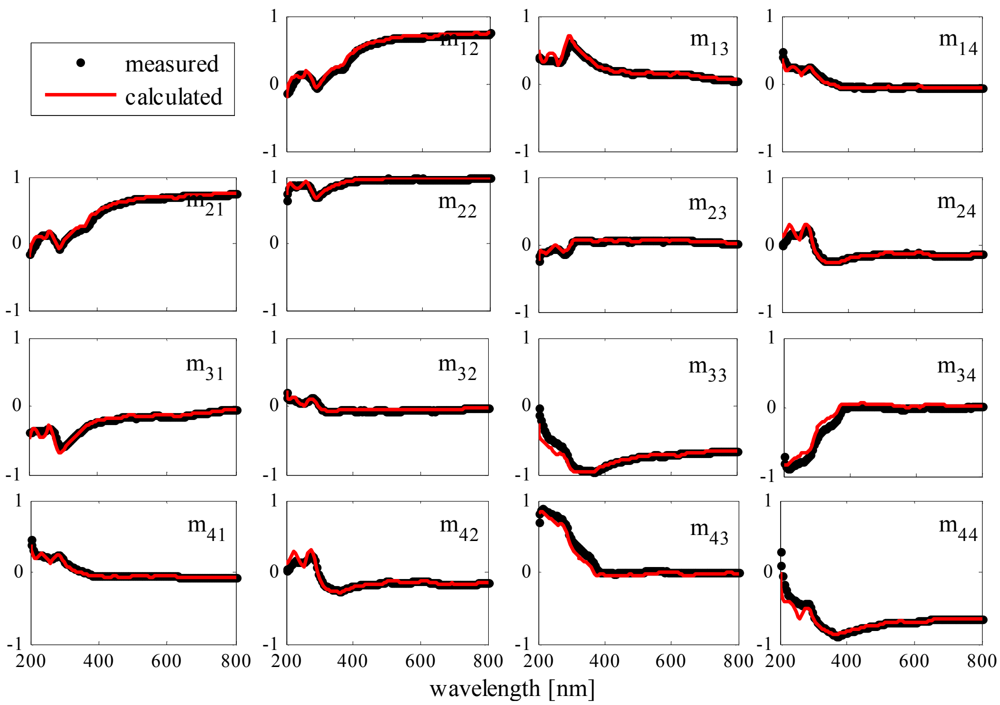

Figure 11. Example of the measured and best fitted (calculated) Mueller matrices for the silicon grating at the azimuthal angle of 60° and incidence angle of 75°.

6. CONCLUSIONS

Computational metrology refers to a measurement method where a complicated measurement process is modeled as a forward problem and some measured data are obtained by a specific instrument under a certain measurement configuration, and then the measurands are precisely and accurately reconstructed by solving the corresponding inverse problem. The fundamental concepts, key issues, and their generalized solution methods of computational metrology are explored in this paper, with the emphasis on the significance and necessity to apply modern mathematical theories and tools in solving the related problems. Some case studies are presented and have demonstrated the efficiency and feasibility of computational metrology. It is expected that computational metrology will provide a fast, low-cost, non-destructive, and accurate measurement in high-volume nanomanufacturing.

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