THE CHARACTERIZATION OF GRATINGS USING THE OPTICAL SCATTEROMETER

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A technique for characterizing gratings, the optical scatterometry, is presented under its both aspects: experimental and theoretical, the way we practice it at the *National Institute for Laser, Plasma and Radiation Physics* (NILPRP). We present the simple and versatile, precise and capable of complex types of ellipsometric measurements scatterometer that we built at NILPRP together with an example of application for estimating the parameters of a grating. All the prominent features of a scatterometric application are touched: the mechanical and optical design of the measuring device, the remote operating software, the diffraction theory for interpreting the data and the error and sensitivity analysis with stress on the original contributions of the authors.

Key words: scatterometry, gratings, ellipsometry, diffraction theory, measurement.

1. INTRODUCTION

The development of the microelectronics/nanolithography industry has created the need for reliable metrology techniques for the characterization of the microstructures and nanostructures. Critical elements of these small structures, such as the *Critical Dimension* (CD), the reproducibility and the uniformity of the structures are areas of concern. Contact metrologies such as *Atomic Force Microscopy* (AFM), and non-contact metrologies such as scanning electron microscopy (SEM) and scatterometry [1–12] were developed to fulfil this need. Among these techniques, scatterometry has the advantages of being non-contact, non-destructive and not requiring special environmental conditions such as vacuum.

Scatterometry is an optical metrology technique designed for the characterization of the test samples from lithography. A typical test sample is represented in Fig. 1. It is a diffraction grating with linewidth *lw* having the same value as the lithographic CD. The linewidth is the most important parameter of the sample to be determined. The light that is back-diffracted by the grating consists

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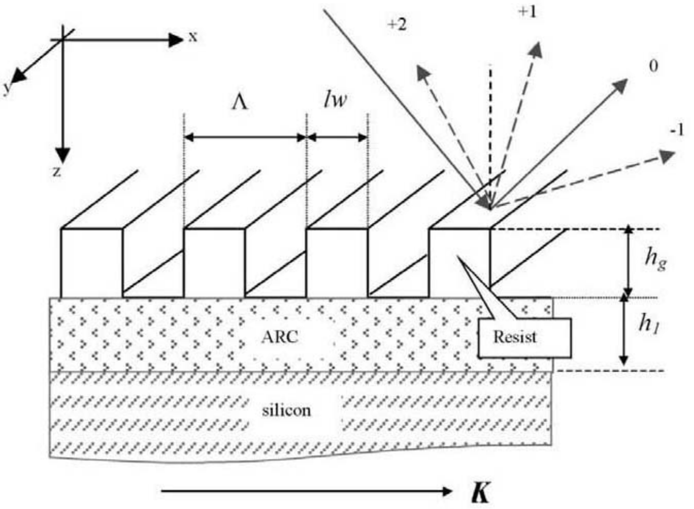

Fig. 1 – A typical grating sample and the diffraction problem.

generally in multiple orders. Because the zeroth order is generally the strongest is usually the only one that is measured. Also, in the conditions of the continuous miniaturization trend in the nanolithography industry, this order is oftentimes the only one available.

Also gratings are at the core of numerous scientific and technological recent advancements such as photonic crystals, liquid crystals displays, *Anti-Reflex Coating* (ARC), etc.

For the above reasons, as well as for fundamental research on the physical properties of gratings, we built at the *National Institute for Laser, Plasma and Radiation Physics* (NILPRP) a variable angle scatterometer of our own, comprising all the elements that define such an instrument: mechanical design that allow for the automatic variation of the incidence angle range of the sample holder and the corresponding adjustment of the detector position, spatial filter and focusing optics, optical measurement device, software for operating the hardware and software for processing the data, polarizer, analyzer and phase retarders for controlling the polarization state of the beam incident onto the grating and the outgoing beam respectively. Not all the components mentioned above have the same importance for the functioning of the scatterometer. Some are mandatory, such as the mechanic structure, which is basically a goniometer, others are strongly recommended, such as software control and spatial filtering, and others are optional, such as the polarization components.

This work is a continuation of the work started at the University of New Mexico, USA, under the leadership of professor John R. McNeil [1–9].

2. EXPERIMENTAL ARRANGEMENT

The blueprint of the scatterometer, a computer assisted design of the scatterometer is shown in Fig. 2, except for the rotator of the detector that cannot be seen from that view. The detector rotator is shown in Fig. 3. Also the optional and the strongly recommended components are not shown for reasons of simplicity and clarity. Only the mandatory components are shown. Basically the scatterometer is an ellipsometer that takes into account the existence of the multiple diffraction orders generated by gratings as seen in Fig. 1, and is able to measure all the nonevanescent ones.

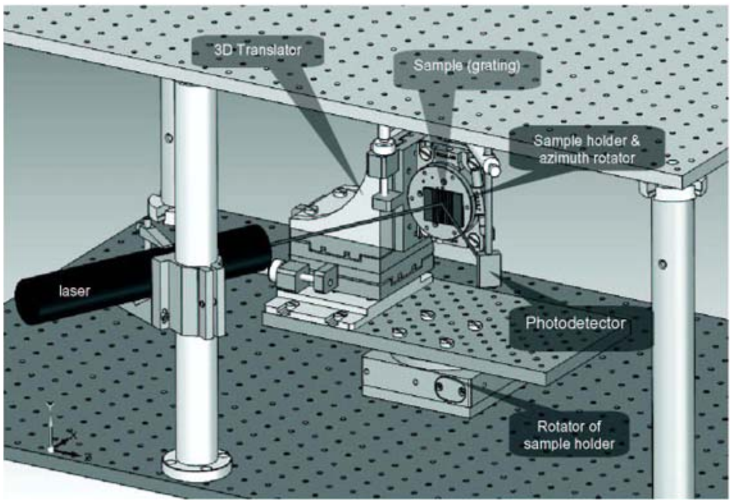

Fig. 2 – The blueprint of the scatterometer consisting in the mechanical design and ellipsometric function. Not shown in the figure for reasons of simplicity and clarity are the spatial filter, which, if existent, would be placed immediately in front of the laser in the path of the laser beam. Following the spatial filter one may insert a lens to focus the beam onto the grating. Between the lens and the grating one can insert a polarizer and maybe a phase retarder for controlling the polarization state of the incident beam. In order to control the polarization state of the beam whose intensity is measured by the photodetector, an analyzer and maybe another phase retarder may be introduced between the grating and the photodetector.

The alignment is a critical issue in great part due to the fact that all photodetectors have a non-uniform sensitivity across their surface and therefore a scatterometrist must make sure the ray diffracted by the grating hits the same spot on the photodetector surface. The detector arm and the sample holder must be perfectly aligned and they have to be in perfect sync. Also the ray coming from the light source must hit the grating in the same spot so that the eventual nonuniformity of the grating will not affect the consistency of the measurement. More so when the purpose of the scatterometrist is precisely to assess the uniformity of the grating and he/she needs to determine the parameters of the grating in various regions of its area and not an average across the whole grating.

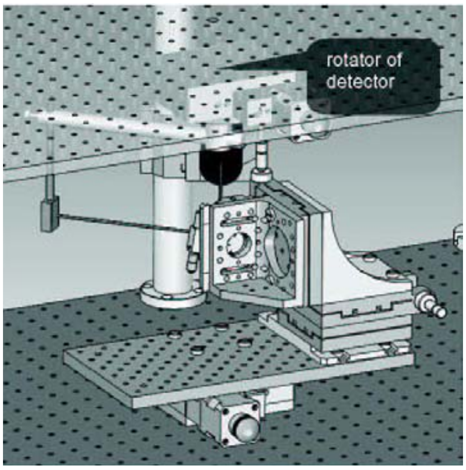

Fig. 3 – Close view of the detector rotator from the opposite side of Fig. 2’s view.

Another experimental issue that has to be dealt with is the central control and command of the various parts of the scatterometer. For this purpose we wrote a Labview code, *i.e.* we created a virtual instrument (VI) that moves in sync the mobile parts of the scatterometer, takes the measurement and continue with the next step, that is the next programmed incident angle. In Fig. 4 we have a picture of the panel of the VI that controls and commands our scatterometer.

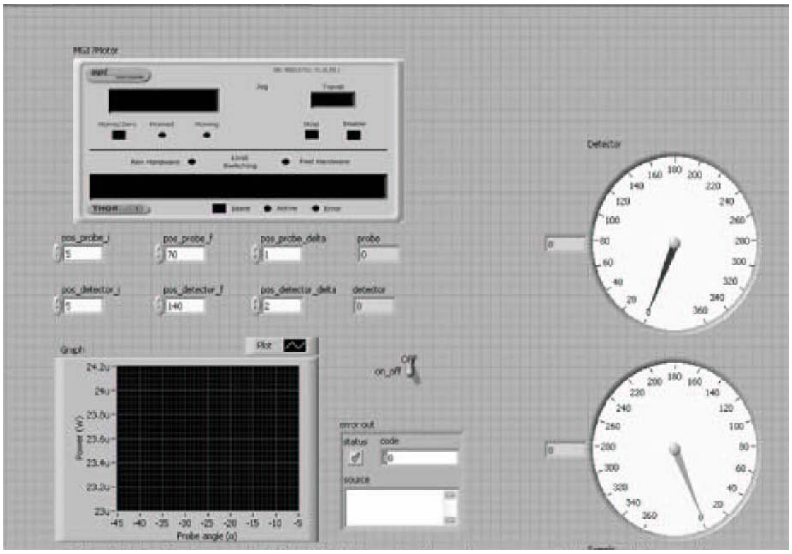
pos_probe_i 5
pos_probe_f 70
pos_probe_delta 1
probe 0
pos_detector_i 5
pos_detector_f 140
pos_detector_delta 2
detector 0
code 0

Fig. 4 – The front panel of the VI that controls and commands the scatterometer.

The measurand is of ellipsometric type and, with the proper adjustment of the polarizer and the analyzer and eventually phase retarders, it can be the power reflection coefficients Rpp, Rsp, Rps and Rss or the squared absolute value of a linear combination of the field reflection coefficients rpp, rsp, rps and rss [8,9]. The measurand is a function of 7 independent parameters, the 4 amplitudes and 3 of the phase differences of the field reflection coefficients with respect to the fourth. There are only 3 independent phase parameters because the 4 phases contain an arbitrary additive phase shift and only the difference of 2 phases has meaning.

3. DATA PROCESSING

As opposed to the experimental simplicity of scatterometry, the data processing is very complex, time-consuming and requires a separate discussion for each of its aspects: the diffraction theory, the software implementation and the optimization of the sensitivity. The contemporary spectacular improvement and continuous growing of the computers performance makes the transfer of the burden of complexity from the experimental to the computational pole very suitable in terms of costs and precision. It should be mentioned at this point that the bulk of original contributions of the authors to data processing is concentrated in the sensitivity optimization area.

3.1. DIFFRACTION THEORY

There is a variety of diffraction theories that may be used to model the diffraction of light on gratings [13]. In our lab we use a code based on the *Rigorous Coupled-Wave Analysis* (RCWA) as outlined in references [14,15] with the improved convergence modification [16]. This diffraction theory is particularly suited for computer implementation and works for a variety of grating line shapes by using the slicing technique. The slicing technique consists in modeling the profile of the grating element as a stack of rectangular slices. This operation is necessary because by construction RCWA can work only with rectangular profile, which is of course a drawback, but it also what makes possible RCWA. In past formulations of RCWA due to the slicing the computation time was increasing approximately exponentially with the number of slices. We use an improved formulation [14,15] in which the computation time increases only approximately linearly with the number of slices.

There are many theories such as *Modal Analysis* (MA) and the *Coordinate Transformation Method* (CTM) [13] which can be used with various degrees of success and in certain cases they may be preferable to RCWA. For instance the CTM does not require slicing, but of course it has disadvantages of its own, like the fact that requires one to work with transformed coordinates. MA has the advantage that by computing the modes of the grating gives physical insight, but, just as

CTM, requires the solving of a transcendental equation, which makes computer implementation difficult. The complexity of RCWA and other diffraction theories, despite their continuous improvement over the years, causes one of the main difficulties of scatterometry, the long computation time of theoretical values of the measurand needed for comparison and fitting to experimental values.

3.2. SOFTWARE IMPLEMENTATION

The software implementation aspect of the data processing includes the conversion of the diffraction theory in code lines, the fitting procedure of the theoretical to experimental data and computation speed issues. RCWA is already optimized for computer implementation. As a fitting procedure we used the Levenberg-Marquardt algorithm [17], which is quite fast, being a gradient type search algorithm, but it is also robust, avoiding local minima. The problem of the timeconsuming calculations is partially solved by using a multithread architecture of distributed computing that uses for each thread a different core or processor of the local computer network.

3.3. SENSITIVITY OPTIMIZATION

Due to the miniaturization process the periodic structures that we characterize become smaller and smaller. For this reason the sensitivity of the measurement, i.e. the change of the measurand with respect to changes of the grating parameters has to be optimized.

The simplest way to improve the measurement sensitivity is to use shorter wavelength light sources. And today there are scatterometers that work with UV or even deep UV lasers [10]. The problem is that such lasers are expensive and the necessary accompanying optics is expensive too and worse, less precise than the optics for visible light. Our scatterometer works for now with He-Ne, 633 nm wavelength laser but in the future we might add additional light sources of shorter wavelength.

Another way to improve the sensitivity is the application of the Sensitivity Analysis for Fitting (SAF) algorithm [8]. The algorithm consists in finding the experimental configuration that yields the best measurement sensitivity. The way it does this is a double process of counteroptimization of the sensitivity with respect to the assumed range of grating parameters for a certain measurement configuration and the choosing of the configuration with the optimum sensitivity calculated under this conditions. It can be said that SAF is a worst scenario procedure, one that provides a measurement configuration that is not only sensitive but also stable with respect to the grating parameters. The order of the application of the processes in which consists SAF is very important. Were the order inversed the result would be meaningless. SAF is one of the most representative and important contribution of the authors to scatterometry. SAF is not, obviously, the only optimization algorithm, not even the only one used in scatterometry [11].

If SAF is a sort of “brute force” approach, because it makes no educated guesses and is designed to work in any situation and it can optimize any measuring devices, the search for Wood-type anomalies of the grating and the use of their property to greatly enhance the sensitivity if one measures at experimental parameters where the anomaly occurs (specific pairs of azimuth angle φ and incidence angle θ) might be considered a “smart” approach [12]. The “smart approach” may help one finding the optimum measurement configuration very quickly, but it has the disadvantage that is not always working because it is contingent upon the existence of such useful anomalies. This is again one important contribution of the authors to scatterometry, one that promises new developments for the future, not only in the domain of scatterometry sensitivity but also of fundamental physics.

4. CONCRETE EXAMPLES

In Fig. 5 there is an illustration of the determination of the unknown geometrical parameters of a grating sample by fitting experimentally measured scatterometric data to theoretical data generated using RCWA. The analyzed sample consists in a grating made out of resist on top of an ARC layer on top of the silicon substrate. The measurements were taken in the optimum measurement configuration corresponding to this particular sample, configuration found using the SAF

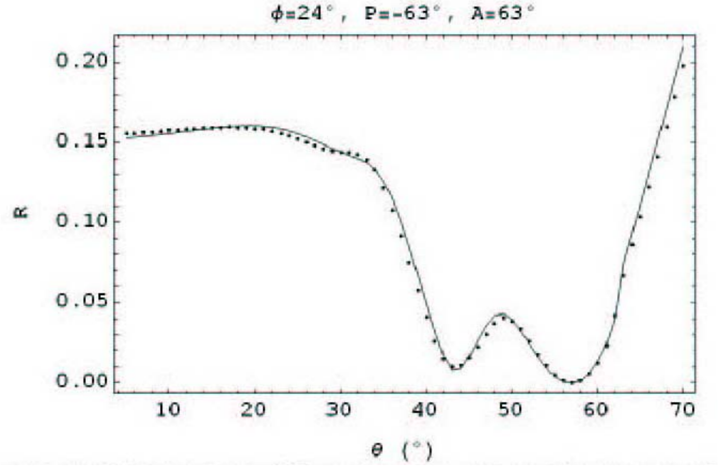

Fig. 5 – Example of fitting experimentally measured scatterometric data to theoretical data generated using RCWA.

algorithm. The optimum configuration consists in the set of three experimental parameters shown in the top label of Fig. 5, and is azimuth $\varphi=24°$, polarizer orientation angle $P=-63°$ and analyzer orientation angle $A=63°$. The angles were measured from the p axis of a system of coordinates type “ray-coming”, which determines the sign of the angles values too. The parameters of the sample are illustrated in Tables 1 and 2, corresponding to the parameters determined using non-scatterometric and scatterometric means respectively. Since the fitting procedure increases exponentially in complexity, it is preferable to know a priori as many as possible of the sample parameters before the fitting of the scatterometric data. For instance the pitch of the grating may be determined from the angular position of the diffracted orders and the refractive indices of the component materials may be determined independently using ellipsometric measurements of the said materials in bulk state. The parameters from Table 1 are also needed for use in the fitting procedure which yields the parameters from Table 2.

Table 1

Parameters of the analyzed sample determined by non-scatterometric means

Parameters→	pitch Λ (nm)	n resist	n ARC	n Si
Values→	438.4	1.64	1.66	3.882 – i 0.019

Table 2

Parameters of the analyzed sample determined by scatterometric means

Parameters→	linewidth lw (nm)	height resist h_g (nm)	height ARC h_1 (nm)
Values→	146.8±0.7	567.0±1.0	159.4±0.6

The errors shown in Table 2 are uncertainties. They illustrate the degree of reproducibility of the results. In themselves, without reference to other results in the field, they are remarkable. They are in the subnanometer range, where the properties of the matter become exotic and often unpredictable. It is a matter of philosophical debate whether subnanometer measurement uncertainty has physical meaning. If true, this degree of precision is more than adequate for the need of precise characterization of the grating parameters. In the error budget of the uncertainties from Table 2 only contributions from random type of errors enter. Such errors are the power fluctuations of the laser, random positioning errors of the sample holder and the detector arm, random variations of sensitivity across the photodetection surface, random fluctuations of the position of the light spot on the grating, in an inextricable mix. It is hard to tell with what percentage each of these possible source of errors contribute to the total error. A more serious problem is the systematic errors. Each of the sources of random errors mentioned above may be also sources of systematic errors, but there are others too. For instance an incorrect working model for the grating element profile can compromise the theoretical data generated by the RCWA code. Another possible source of systematic errors is the fact that the parameters considered as known, the refractive indices in particular, are generally measured using bulk materials, and matter structured at the nanoscale may not have the same properties as the bulk matter. One may be aware of the existence of systematic errors by using different measurement configurations for estimating the grating parameters. Each configuration is affected differently by the systematic errors, and, if the different configurations yield values for the grating parameters that are separated by more than their combined uncertainty, this is a sure sign of systematic error. And in practice we were confronted often with this situation. The truth is that the uncertainty may be improved indefinitely and indeed there are claims of reaching subpicometer uncertainty in dimensional characterization [18]. On the other hand sobering reports show that with even the best technology available one cannot reach an absolute accuracy better than 10 nm [19]. At this point one may ask what is the point of improving the estimation uncertainty, as we have done, when the systematic errors are already larger than the uncertainties for non-optimized systems. There is a pragmatic answer for this question and this is the best we can do for now: the nanolithography industry is less interested to know exactly the dimensions of the structures they built than how well and how uniform those structures may be reproduced. And to this interest of the industry we can offer a very precise solution.

5. CONCLUSION

Scatterometry is an optical metrology technique designed to characterize the parameters of lithographic test samples. Because it is an optical metrology, it is non-contact and nondestructive. At NILPRP we built a scatterometer based on an original design, both the mechanical and the software part that a scatterometer comprises. This work was a continuation of the work started at University of New Mexico, USA, under the leadership of professor John R. McNeil. Scatterometry also has a great potential for improvement due to the large domain of the available measurement configurations to choose from. In this area we concentrated our research looking for way of optimizing the sensitivity of the measurement configuration. The sensitivity of scatterometry can be improved alternatively using physical phenomena such as Wood-type anomalies resonances and by using light sources of shorter wavelength, but also using a scanning procedure such as SAF, which analyzes the domain of possible measurement configuration for an assumed range of grating parameters and yields the optimum configuration. Scatterometry is able to satisfy the metrology needs of today's and tomorrow's lithography and it creates opportunities for contributions to the fundamental physics of gratings, such as the analysis of Wood-type anomalies.

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