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Novel optical metrology for inspection of nanostructures fabricated by substrate conformal imprint lithography

Teun D G Nevels[1], Lieke J M Ruijs[2], Paul van de Meugheuvel[2], Marc A Verschuuren[2], Jaime Gómez Rivas[1] and Mohammad Ramezani[1,3,*]

[1] TeraNova B.V., Groene Loper 5, 5612AE Eindhoven, The Netherlands
[2] SCIL Nanoimprint Solutions, High Tech Campus 11, 5656AE Eindhoven, The Netherlands
[3] Institute for Photonic Integration, Department of Applied Physics, Eindhoven University of Technology, P.O. Box 513, 5600 MB Eindhoven, The Netherlands

E-mail: m.ramezani@tue.nl

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Abstract

Substrate conformal imprint lithography (SCIL) technology enables the fabrication of complex and non-trivial 3D nanostructures such a slanted gratings and metasurfaces with sub-10 nm resolution over large areas for industrial-scale production, which can be fabricated in a single lithography step. This technology utilizes novel composite silicone rubber stamps that provide versatility in addition to high precision. To inspect the quality and reproducibility of the nanostructures that are fabricated using SCIL, a novel optical characterization method using Fourier microscopy is proposed. In this method, nanostructures are illuminated under a microscope objective using a collimated light beam at different incident angles and the properties of the reflected and/or diffracted beams are analysed to extract the critical dimensions of the nanostructures. This fast and non-destructive method has the potential for being used as an in-line inspection technology to extract the critical dimensions of the nanostructures over large areas and improve the overall properties of nanostructured surfaces.

Keywords: substrate conformal imprint lithography, grating, Fourier microscopy, scatterometry, metrology

(Some figures may appear in colour only in the online journal)

1. Introduction

The ability to fabricate micro- and nano-scale patterns in a cost-effective manner on wafers up to 300 mm is required for many novel applications. Especially, the direct patterning of functional optical material without the need for complex and iterative deposition and etching steps is highly relevant to meet the cost and throughput requirements for the fabrication of nanophotonic components for consumer applications [1]. Within the field of nanophotonics, these structures are key in the development of more efficient lasers, solar cells, and LEDs [2–4]. Other important applications of these nanostructures are virtual and augmented reality (VR/AR) technologies, which have attracted an increasing amount of attention over recent years [5]. All these applications rely on compact optical devices based on gratings and metalenses that can be made using different nanofabrication methods and processes [6]. Within these nanofabrication processes, nanolithography is a critical method which refers to a group of technologies

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that is used to pattern large-area wafers with nanometre precision. Nanoimprint lithography (NIL) and UV-lithography are two examples of nanolithography technologies [7]. While UV-lithography is used for the fabrication of semiconductor chips and integrated circuits on an industrial scale, other applications such as AR/VR are fabricated using NIL technology [8]. In AR/VR, often complex 3D structures with strict size and roughness constraints are used. These structures can be fabricated using NIL in a more straightforward manner due to the versatility and precision of this method.

After the nanopatterning, quantifying the optical properties of the nanostructures is a critical step to maintain the quality of the samples. Many different approaches can be utilized for this purpose. Among these, visual inspection, scanning electron microscopy (SEM), atomic force microscopy (AFM), and scatterometry are the most common methods [9, 10].

In this work, we first describe the principles of NIL technology and how this method can be utilized for the fabrication of complex geometrical nanostructures. In the second part of this work, we explain a novel scatterometry method based on Fourier microscopy that is able to quantify the geometrical properties of periodic nanostructures by combing the experimental results with simulations. In this approach, we use a collimated light beam to illuminate the nanostructures under well-defined angles of incidence, allowing us to measure several diffraction orders over a wide range of detection angles simultaneously. This configuration, in combination with simulations, results in determining the geometrical properties of nanostructures with resolutions as high as 3 nm and over large areas. This approach distinguishes itself from other works in the literature on Fourier scatterometry, in which the phase difference properties are investigated using a focused beam spot [11–13].

2. Direct patterning of optically functional inorganic materials

The possibility to fabricate functional optical surfaces using inorganic materials is critical in AR/VR and metasurface applications [6, 14]. Conventional methods for the fabrication of nanostructures are photolithography, electron-beam lithography, and NIL [1]. Although scanning beam lithography is a very accurate method, which can be used to fabricate complex nanopatterns with high resolution, this method is very slow and expensive for industrial applications [15]. Photolithography, on the other hand, is able to pattern large areas, but is not able to pattern structures with complex shapes in a single lithography step, leading to several iterative lithography steps to achieve complex geometries [16]. Finally, NIL is able to pattern relatively large areas with complex nanostructure shapes in a single lithography step. However, this method is limited in resolution and defect control due to the use of a stamp [17].

NIL was first introduced using rigid stamps. This approach suffered from intrinsic issues due to the stiffness of the stamp. Introducing soft imprint lithography, that uses a soft stamp made from poly-di-methyl-siloxane (PDMS), established a method that is able to make conformal contact over large areas in a cost-efficient, effective, and high throughput manner. Moreover, this method has the advantage of being insensitive to particle contamination or stamp release with respect to NIL using rigid stamps [18]. Despite several advantages of imprinting using soft stamps, the inability to imprint features with nanometre resolution is the main disadvantage of this method. This limitation arises from the ability of the rubber features to collapse, which is due to their flexibility and tendency to deform under the influence of surface tension [17].

Substrate conformal imprint lithography (SCIL) is a distinct approach in NIL, which uses a composite stamp consisting of two rubber layers supported by a glass layer. This stamp is flexible in the out-of-plane direction and stiff in the in-plane direction, which results in the following two characteristics: (a) possibility of making conformal contact on areas as large as the surface of a 300 mm wafer, and (b) preventing distortions in the pattern due to the stiffness in the in-plane direction. Due to the flexibility of this stamp, only a minimum pressure of approximately 20 mBar is required to imprint nanopatterns, which prevents damage to both the structures and the stamp. Moreover, due to this flexibility, the method is not susceptible to inducing damage by contamination since the pattern is imprinted over the contaminants and leaves the surrounding pattern undisturbed. Altogether, SCIL solves the limitations of conventional NIL and is able to replicate complex patterns with nanometre resolution over large areas in a time- and cost-efficient manner [15, 17].

2.1. Direct patterning of complex patterns

A schematic representation of the steps involved in SCIL fabrication is shown in figure 1. First, a PDMS stamp containing the inverse replica of the desired structure is prepared (figure 1(a)). The PDMS stamp is made from a master that contains the desired pattern by first pouring liquid silicone rubber over it and then thermally curing the silicone at 50 °C. Thereby, the stamp adopts the inverse replica of the desired pattern. Subsequently, the stamp is applied to a layer of sol-gel resist (inorganic imprint resist) through which capillary forces assist to fill the stamp with the resist (figures 1(b) and (c)). After the stamp has been fully filled, the liquid starts forming a silica-like network due to the silicon oxide precursors that are present in the resist (figure 1(d)). After the resist is solidified, the stamp is released, and a replica of the master pattern is fabricated onto the substrate (figure 1(e)).

PDMS-based nanoimprinting with an organic resist does not allow for high-volume production due to the limited stamp lifetime, variations in duty cycle (DC) due to resist-stamp interaction, and oxygen-inhibited slow cure. Moreover, organic resists are light-sensitive and susceptible to relatively high temperatures, which are conditions that might be applied in the end-user applications. Alternatively, inorganic materials are stable under these conditions, hence they can be directly used for optical applications. SCIL is able to pattern fully inorganic resists. As shown in figure 1, these inorganic materials are made through a sol–gel method which provides an inorganic based crosslinking route for replication of patterns

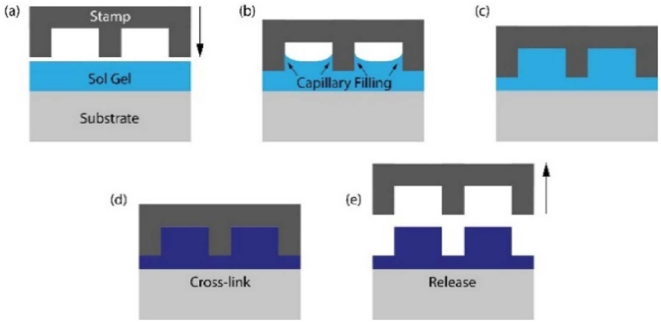

Figure 1. Schematic representation of the steps involved in SCIL using inorganic sol–gel resist.

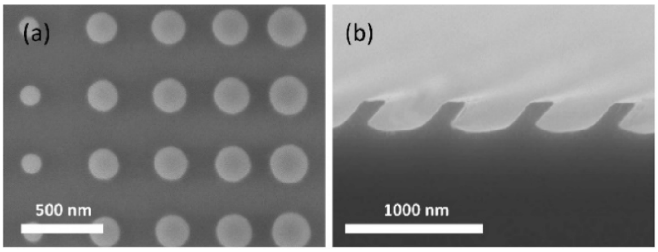

Figure 2. SEM images of examples of nanostructures that are fabricated by SCIL: (a) a top-view of a metasurface and (b) a cross-sectional view of a slanted grating.

without the need of UV radiation, which is commonly used in other NIL techniques [15].

Using the straightforward approach that SCIL offers, we can fabricate complicated geometries in a simple manner. SEM images of two different structures with complex geometrical shapes that are fabricated using SCIL are displayed in figure 2. Figure 2(a) shows a top-view of a metasurface that consists of several pillars with different diameters in one unit cell. Figure 2(b) shows a cross-sectional view of a slanted grating. Slanted gratings are 1D gratings of which the profile is tilted in the vertical plane (i.e. negative angle). These gratings provide additional freedom in the design of the optical properties. With a proper choice of dimensions, approximately all the light can be directed into one diffraction order, while all other orders are suppressed. This property is of particular interest for AR applications, in which the gratings are used close to the user's eye. The flexibility of the stamp used by SCIL aids in the demolding and releasing of the patterns with negative angles (figure 2(b)). The fabrication of slanted gratings is carried out in one step with SCIL, while using conventional photolithography and dry etching methods (under which the wafer is tilted during the dry etching step), such structures require separate lithography and etching steps for each pattern. Nevertheless, the stamp release for slanted gratings is more complicated since the PDMS stamp must be deformed considerably to prevent defects in the fabricated grating.

In applications such as AR, both precision and reproducibility with nanometre accuracy are required for the fabrication of nanostructures [6]. State-of-the-art SCIL can provide such levels of fabrication precisions in high-volume production. However, a rapid in-line quality inspection method for such complex patterns is required to monitor the SCIL process, to verify the sample quality, and to ensure the reproducibility.

3. Optical characterization using Fourier microscopy

One of the important steps within nanofabrication is the non-destructive quality inspection of the fabricated nanostructures with a high throughput. Currently, the methods that are used for characterizing nanostructures are mainly limited to SEM and AFM [9]. One of the major drawbacks of these methods is their destructive nature: to extract cross-sectional parameters, one needs to break the sample. Therefore, these techniques cannot be integrated into a production line for high-volume inspection of samples. Moreover, the slow measurement time of these techniques is another important limitation. Additionally, methods such as SEM and AFM are only suitable for finding single and localized defects across the samples. However, for many nanophotonic applications, such as AR glasses, single defects are not detrimental, and measuring the critical dimensions of the features over large areas is more important. Moreover, nanostructures fabricated by methods such as SCIL are susceptible to changes in the refractive index, which cannot be characterized using the conventional characterization methods. Therefore, the quality inspection method must be able to characterize both the optical performance and the geometrical parameters of nanostructures in a non-destructive manner.

To address the need for quality inspection for characterizing the critical dimensions of gratings, we have developed a fast and non-destructive technique, which is able of quantifying the critical dimensions of fabricated gratings (with a pitch as low as 310 nm) with nanometre accuracy. This technique is based on Fourier microscopy and quantifies the intensity and the angle of diffracted orders that are generated by illuminating a grating at well-defined angles of incidence. Unlike other Fourier scatterometry methods described in literature, which use a focused beam spot, this technique uses a collimated laser beam (405 nm) that illuminates the nanostructures (inspection diameter 100 μm) through an objective lens (achromat, numerical aperture (NA) 0.8, working distance 0.3 μm) [11–13, 19]. This collimated illumination is realized by focusing the incident laser beam in the back-focal plane of the objective lens. By scanning the position of the focused light on this plane, the incident angle on the grating is adjusted. The measurements can be performed for both transverse electric (TE) and transverse magnetic (TM) polarization within the angular range determined by the NA of the objective lens. The diffracted orders are collected as a function of the incident angle by the same objective lens and are subsequently focused into the back-focal plane of the objective lens and imaged on a charge-coupled device (CCD) camera. The principle of this technique is schematically illustrated in figure 3. In this figure, the zeroth (blue) and first (red) diffraction orders are collected by the objective lens as their diffraction angles are within the NA of the objective lens, while the second order diffraction (green) is not collected. By introducing a lateral shift in the position of the focus of the incident light in the back-focal plane (Δ),

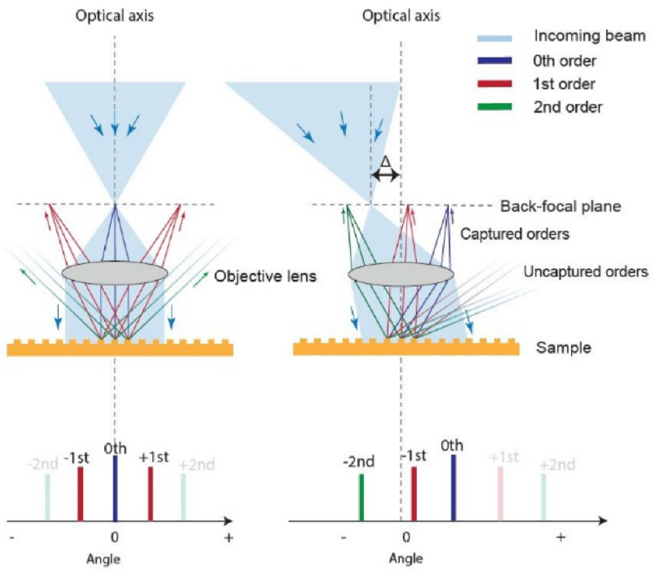

Figure 3. Schematic representation of the optical scatterometry technique in which a collimated laser beam illuminates a grating at well-defined angles, which are determined by the shift of the focus spot of the incident wave in the back-focal plane of the objective lens with respect to the optical axis (Δ). The captured orders of diffraction in the back-focal plane are represented by intensity peaks at the respective angles.

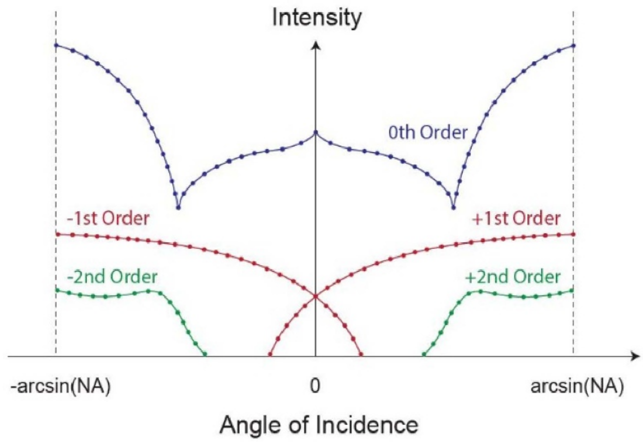

Figure 4. Illustrative example of the optical response of a grating measured as a function of the angle of incidence. The captured zeroth, first and second diffraction order are shown in the angular range determined by the numerical aperture of the objective lens.

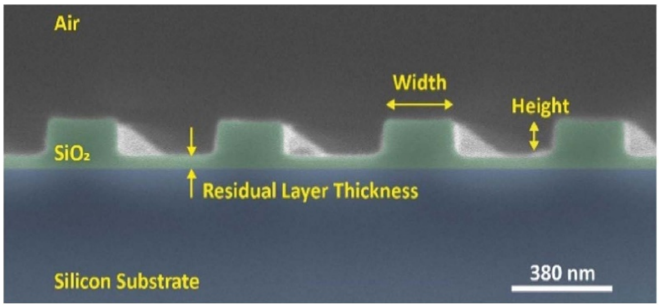

Figure 5. SEM cross-sectional image of the optical grating, including a representation of the different geometrical parameters, such as the height, width and residual layer thickness (RLT).

the incident angle is modified, and the intensities and angles of the diffracted orders are changed accordingly. The approximate diffraction angle can be calculated using Bragg's grating equation:

$$\alpha\left[\sin\left(\theta_m\right)+\sin\left(\theta_i\right)\right]=m\lambda,$$

where α is the pitch size of the grating and θ_m and θ_i are the diffraction and incident angles, respectively. In this equation m ($m = 0, \pm1, \pm2, \ldots$) determines the order of diffraction and λ is the wavelength of the incident light. With this technique, we can evaluate the relative intensities of different diffraction orders that are supported by the grating. A schematic illustration of the optical response of a grating is shown in figure 4. This figure shows the intensities of the zeroth (blue), first (red), and second (green) diffraction orders as a function of the angle of incidence. The optical response shown in figure 4 is unique for a nanostructure with a set of geometrical and optical parameters. Consequently, minor modifications of these parameters or inhomogeneities in the samples will affect the measured curves considerably. Moreover, the optical response of the samples that are measured using the Fourier microscope can be accurately simulated with electromagnetic simulation packages such as rigorous coupled wave analysis (RCWA). RCWA is a method for analysing diffraction of electromagnetic waves from periodic structures, i.e. gratings, in a semi-analytical manner [20]. By comparing the measured and simulated data, we can extract the geometrical parameters with accuracies as high as 3 nm.

In the following section, we demonstrate the applicability of our Fourier microscopy technique using collimated illumination for investigating the diffraction properties of two different types of gratings: (a) a grating that is designed to diffract visible light, and (b) a grating that is designed to diffract infrared (IR) radiation. Moreover, we simulate the measured optical response with the RCWA method to extract the relevant geometrical parameters. In the final part of this work, we show how this technique can be used for in-line characterization and quantification of the quality of fabricated gratings on different wafers throughout the production process.

3.1. Estimating the geometrical parameters of gratings

Optical grating: Gratings that are designed to diffract visible light (400 nm–700 nm) have pitch sizes comparable to the wavelength of visible light. Such gratings are used in devices for e.g. AR and photovoltaic applications [3, 5]. To investigate the applicability of our metrology technique for extracting critical dimensions of such gratings, we have measured the optical properties of the grating shown in figure 5. We have characterized this sample with SEM to verify the results obtained by Fourier microscopy. This grating is prepared by NIL and is made of SiO_2 on a silicon substrate. The pitch size of this grating is approximately 380 nm.

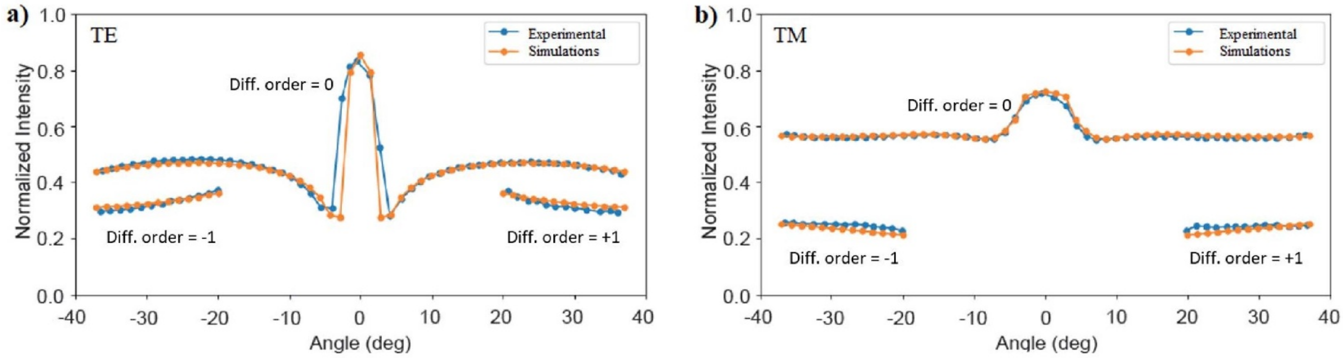

Figure 6. Optical response of the optical grating obtained by Fourier microscopy for (left) TE polarization and (right) TM polarization.

Table 1. Geometrical parameters (pitch, height, RLT and DC) of the optical grating shown in figure 5 obtained by Fourier microscopy and SEM.

	Geometrical parameters			
Method	Pitch (nm)	Height (nm)	RLT (nm)	DC (%)
Fourier microscopy	385 ± 3	102 ± 3	47 ± 3	45.2 ± 0.1
SEM	382 ± 5	97 ± 5	42 ± 5	43 ± 5

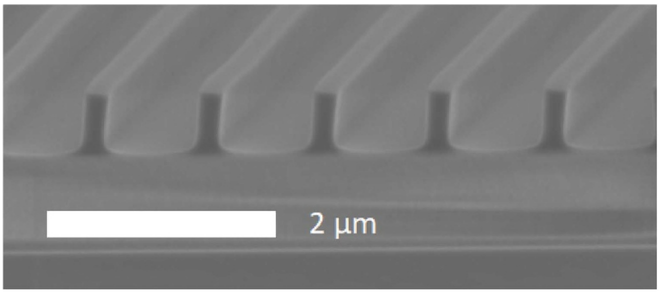

Figure 7. SEM cross section of the infrared grating.

Figure 6 shows the measurements (blue) and simulations (orange) of the normalized intensity for different diffraction orders that are obtained by our Fourier microscopy method. In this method, the sample is illuminated with two distinct polarizations (TE and TM) within the angular range, i.e. between $-37°$ and $+37°$. For both polarizations, the specular reflection (zeroth diffraction order) in addition to the $+1$st and -1st diffraction orders are measured. A typical measurement like the one described, takes approximately 40 s to be executed. Subsequently, the signals for each polarization are normalized by the intensity of the specular reflection from a clean silicon substrate. Thereafter, we can extract the geometrical parameters of the grating from simulated responses that match the experiments, which are obtained by using the RCWA method. We can compare these geometrical parameters with the parameters that are obtained by SEM (see table 1). The SEM that is used for these investigations can estimate the geometrical parameters with ± 5 nm accuracy. As can be seen in table 1, the results obtained by Fourier microscopy perfectly match within the uncertainty to the results that are obtained by SEM.

3.1.1. IR grating. To diffract IR light (700 nm–20 μm), one needs gratings with a larger pitch size in comparison with gratings used to diffract visible light. Currently, to quantify the geometrical dimensions of such gratings after fabrication, methods such as SEM or AFM are used. Here, we investigate the ability of the Fourier microscopy method to measure the optical response of an IR grating and simulate its response to extract the relevant geometrical parameters. For this purpose, we have selected a grating, which its SEM image is shown in figure 7. The grating is made of SiO_2 and is imprinted on a silicon substrate. The pitch size of this grating is 1 μm and it is fabricated by SCIL.

From the SEM image (see figure 7) it can be seen that the geometrical parameters of this grating are considerably larger than those of the optical grating that was investigated in the previous example (see figure 5). The experimental optical response of this grating is shown for both TE and TM polarization in figure 8 (blue). For each polarization, we show the measured signal for the ± 1st diffraction order in addition to the specular reflection (0th order). To extract the geometrical parameters of the grating, the optical response is simulated with the RCWA method at well-defined incident angles between $-39°$ and $+39°$ (orange). In figure 8, it can be seen that an excellent agreement between the experimental and simulated results is achieved for all the captured diffraction orders. From this result, we can extract the geometrical parameters of the grating. These parameters are summarized in table 2 in addition to the values that were extracted from SEM and AFM measurements on this sample.

Due to very large inhomogeneities in the residual layer thickness of this sample and its small area (0.25 mm^2), it was not possible to measure the residual layer thickness with SEM at the exact same position that is investigated by Fourier microscopy. Therefore, we have not reported these values in table 2. Nevertheless, the height and DC of the grating can be measured by both SEM and AFM. The estimated value of the height is in excellent agreement with the values obtained by SEM and AFM. However, the DC shows a larger discrepancy between the different methods. This discrepancy most likely originates from the shape of the grooves. In our simulations, the cross

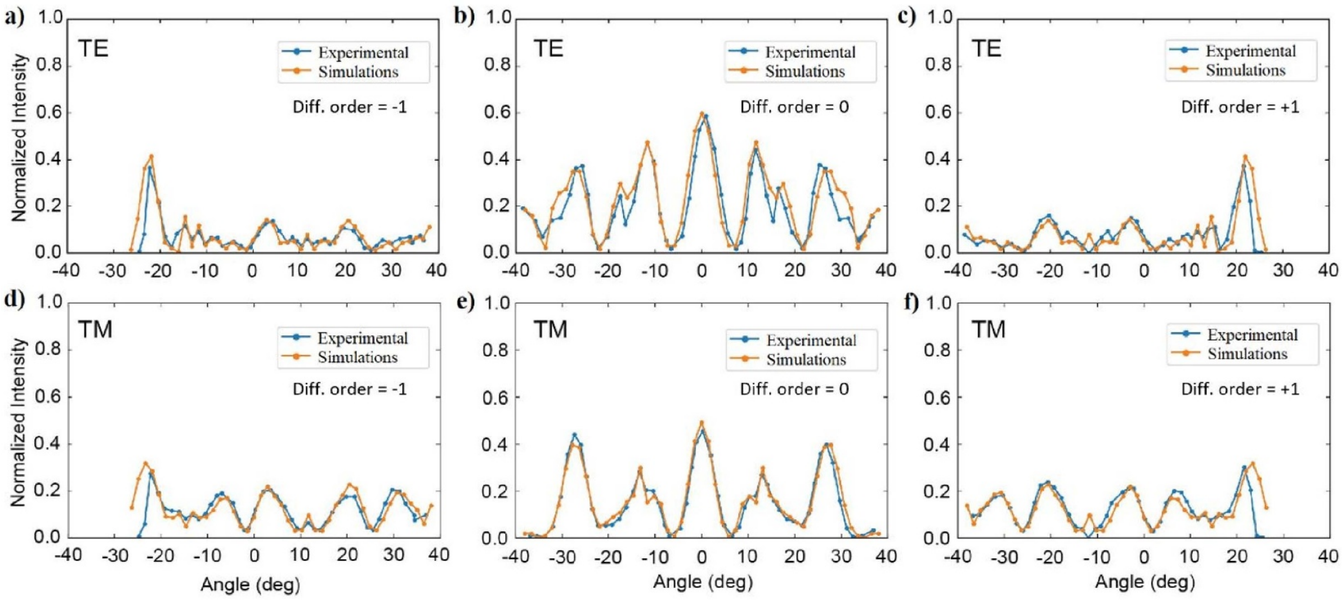

Figure 8. Experimental (blue) and simulated (orange) optical response of the infrared grating for two polarizations TE and TM.

Table 2. Geometrical parameters (height, RLT and DC) of the IR grating obtained by Fourier microscopy, SEM and AFM.

Method	Geometrical parameters		
	Height (nm)	RLT (nm)	DC (%)
Fourier microscopy	539 ± 2	930 ± 2	0.25 ± 0.1
SEM	530 ± 10	N.A.	0.22
AFM	537 ± 2	N.A.	0.21

section of the grooves is considered as trapezoid, while in the SEM image (see figure 7) the grating appears to have a larger curvature towards the residual layer. These features are not yet included in the simulations.

The agreement between experiments and simulations indicates the strength of this metrology method to extract geometrical parameters with a high level of accuracy. Moreover, it shows its scalability and applicability for gratings with distinct geometrical parameters.

3.2. In-line characterization of fabricated gratings

One of the important requirements for high-volume manufacturing of photonic applications is the reproducibility of the fabricated nanostructures. Within this context, the possibility of in-line and non-destructive quality inspection of the samples after fabrication is crucial. Several environmental and operational factors can vary throughout the production. Therefore, a quantitative quality control method that can monitor changes in the uniformity and homogeneity of the samples is critical to improve the fabrication yield. This requirement becomes even more critical when nanometre precision over large area samples (several cm^2) is required. Another important factor to consider is the required time to measure and analyse the samples. Ideally, it is desirable to measure every sample after fabrication and before entering the next processing step. In this section, we show how the Fourier microscopy method can be used as a quick and accurate tool to inspect the quality of gratings. This approach relies on quantifying the difference between the measured optical response of each sample and the reference optical response that is acceptable by the operator. For this purpose, we define a figure of merit known as 'Variation Index (VI)'. The VI quantifies the difference between the sample and the reference (acceptable optical response) according to the following equation:

$$\mathrm{VI} = \frac{1}{N}\sum_{i=1}^{N}\left(\frac{\left|I(\theta_i)_{\mathrm{sample}} - I(\theta_i)_{\mathrm{ref}}\right|}{I(\theta_i)_{\mathrm{ref}}}\right) \times 100.$$

In this equation, $I(\theta_i)$ is the intensity of the diffracted order measured at the angle of incidence θ_i, and N is the total number of data points in each measurement. This metric provides an averaged percentage change between the sample and the reference.

For the purpose of in-line characterization, we have fabricated 25 wafers that contain 1D gratings with geometrical parameters similar to the sample that is described in section 3.1 (optical grating). These samples are fabricated within 2 h of production time using an AutoSCIL 200 tool [21]. The measured optical responses of four of these wafers are shown in figure 9 to illustrate the differences. The measurements are carried out for both TE and TM polarization. In this figure, sample 1 (blue) shows a slightly different response in comparison with the other samples. To quantify these differences, we have calculated the VI of these samples with respect to the ideal optical response. This ideal optical response is determined by measuring the response of a series of identical samples and averaging those responses. The variation of the measurements

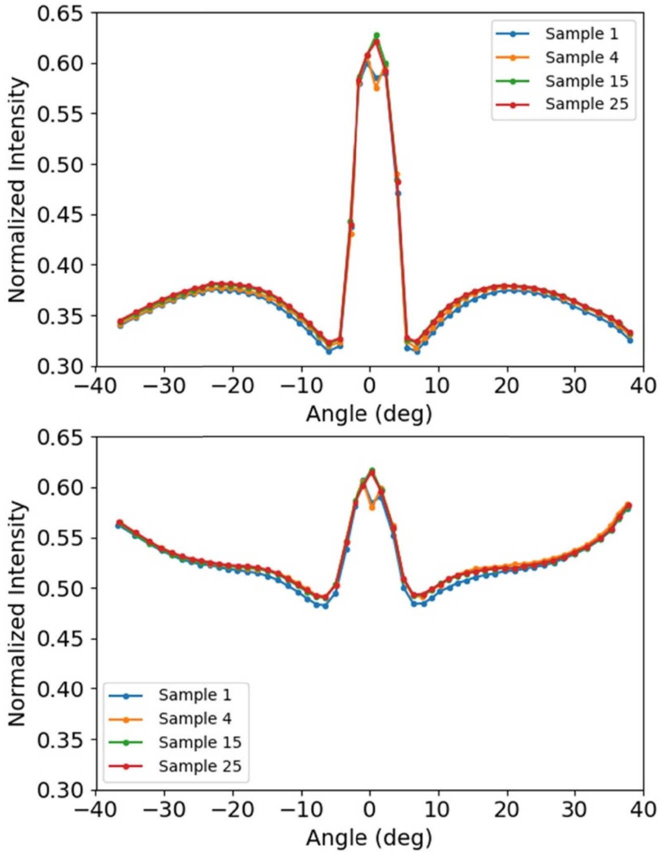

Figure 9. Optical response of four samples among the batch (containing 25 samples) that are measured for two different polarizations (above) TE (below) TM.

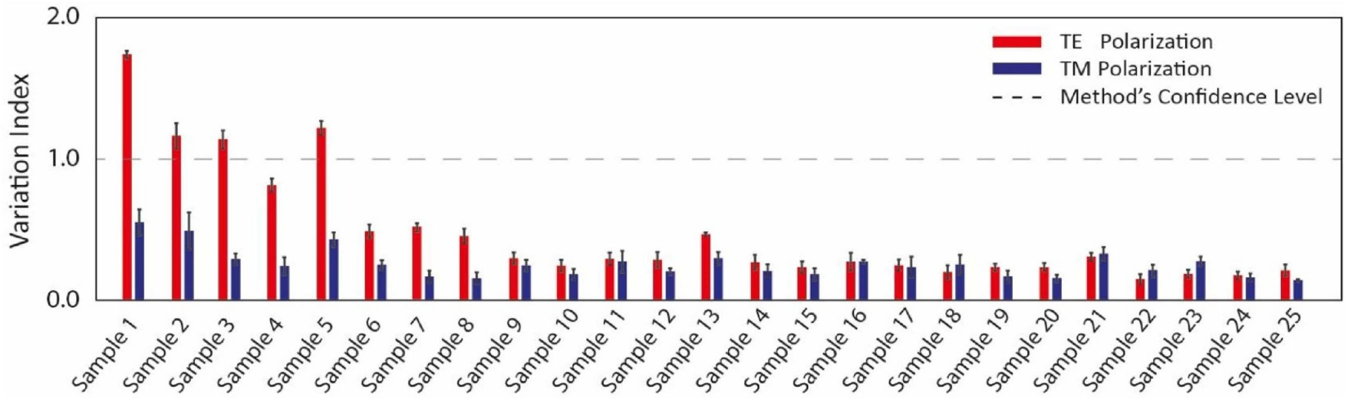

Figure 10. VI of 25 wafers which are fabricated within 2 h of production time using an AutoSCIL 200 tool. The VI is measured for both TE (red) and TM (blue) polarization.

among the ideal samples determines the 'Method's Confidence Level'. Any value above this confidence level indicates a change in the geometrical or physical properties of the sample.

The VI for each of the 25 samples is shown in figure 10. These measurements are repeated four times to test the reproducibility of the measurements. The error bars in this figure represent the standard deviation associated with each measurement. Figure 10 clearly shows that throughout the fabrication process, the optical properties of the first five samples deviate from the subsequent 20 samples. This method of in-line characterization can also be combined with the simulations to determine the origin of the difference in the measurements.

4. Conclusion

In conclusion, we have shown how SCIL technology can be utilized for fabrication of non-trivial nanostructures with complex geometries such as slanted gratings over large areas with nanometre precision in a single lithography step. Moreover, we have demonstrated the potential of Fourier microscopy with collimated illumination for metrology and quality inspection of the nanostructures over large areas in a non-destructive manner. The combination of SCIL technology and Fourier microscopy with collimated illumination provides a powerful method for high-volume production of nanostructures with great reproducibility and precision.

Data availability statement

The data that support the findings of this study are available upon reasonable request from the authors.

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ORCID iD

Mohammad Ramezani https://orcid.org/0000-0002-1863-9123

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