Assessing fabrication tolerances for a multilevel 2D binary grating for 3D multifocus microscopy

Marcelo Davanco, Liya Yu, Lei Chen, Vincent Luciani, and James Alexander Liddle

Center for Nanoscale Science and Technology, National Institute of Standards and Technology, Gaithersburg, MD 20899 USA

Abstract: We perform a comprehensive theoretical assessment of fabrication tolerances for a 2D eight-level binary phase grating that is the central element of a multi-focal plane 3D microscopy apparatus. The fabrication process encompasses a sequence of aligned lithography and etching steps with stringent requirements on layer-to-layer overlay, etch depth and etched sidewall slope, which we show are nonetheless achievable with state-of-the-art optical lithography and etching tools. We also perform broadband spectroscopic diffraction pattern measurements on a fabricated grating, and show how such measurements can be valuable in determining small fabrication errors in diffractive optical elements.

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OCIS codes: (050.1380) Binary optics; (050.1970) Diffractive optics; (050.6875) Three-dimensional fabrication.

References and links

1. Introduction

Diffractive optical elements have been studied for many decades, and nowadays constitute a versatile and highly useful set of tools for optical systems. Elements such as beam-shapers, optical multiplexers and demultiplexers, array generators, spectral shapers and micro-lenses have been demonstrated in the past [1, 2], illustrating the great variety of possible functions that can be made available. A diffractive optical element is in essence an optical element that imparts a pre-determined, spatially dependent phase distribution upon the wavefront of an illuminating optical beam, and thereby determines the diffraction pattern that is formed in the far-field. Synthesis of spatial phase distributions for generating a desired diffraction pattern is typically performed by solving an inverse scattering problem through a numerical optimization routine [2–6]. Phase distributions arising from such routines can be very complicated functions of the spatial coordinates. A popular way of implementing such diffractive optical elements, due to the relatively straightforward fabrication processes involved, is through binary optics. Binary optics are a class of optical elements that consist of a glass substrate with an etched three-dimensional topography, in which the height of the top surface varies in discrete (binary-coded) levels. Level-steps on the glass surface are generated though a sequence of aligned lithography and plasma etching processes, as illustrated in Fig. 1(a) [7, 8]. A larger number of phase step-levels generally translates into a better approximation of the continuous, synthesized phase profile, and will typically lead to elements with superior optical performance; in particular, for blazed diffraction gratings, eight phase step-levels would already produce a maximum theoretical first-order diffraction efficiency of 95 %, and sixteen levels a maximum of 99 %. Fabrication imperfections due to limitations in the lithography and etching processes however lead to performance degradation which can become significant, and so understanding fabrication process tolerances and their dependence on the number of levels is very important in optimizing the diffractive element design for a given process. For example, [10] provides a study of multilevel grating array generators for which layer-to-layer alignment error of the order of one thousandth of a grating period can, alone, lead to a diffraction efficiency drop of about 5 %.

A wide range of approaches have been applied in fabrication of multilevel diffractive optical elements. Contact lithography was historically the primary method used, but projection lithography has gradually become the standard for high quality diffractive optics fabrication, as technical specifications became tighter. Direct-write electron-beam lithography produces excellent results but has well-known drawbacks such as low throughput and high cost, which remain
challenges for process integration and scalability. State-of-the-art optical projection lithography stepper systems, on the other hand, are able to achieve feature sizes of the order of a couple hundred of nm, and sub-100 nm overlay accuracy, with substantially higher exposure throughputs than electron-beam systems. We note also that great effort has also been put toward grayscale lithography and direct laser writing. Grayscale lithography provides good-quality results on multilevel symmetric shape diffractive optical elements, but requires very specialized process development efforts and materials, which make it costly.

In this paper, we theoretically investigate the tolerances required for fabrication of the 8-layer fan-out diffractive optical element demonstrated in [11], and show that such tolerances can be met, though generally with relatively small margins, with the commercially available, state-of-the-art projection lithography and etching tools available in our laboratory. We point out that, whereas the array generators in [10] had unit-cell dimensions of the order of hundreds of microns, requiring alignment error tolerances on the order of hundreds of nanometers - already achievable in projection lithography systems at that time - the fan-out grating in [11] had unit-cells that were smaller by at least an order of magnitude; following [10], this would require alignment tolerances of the order of tens of nm, a result which we verify in detail below. Our investigation emphasize the fact that, whereas electron-beam lithography is traditionally used to fabricate such elements, modern, high-throughput projection photolithography tools can be employed and produce high quality results.

Our fan-out optical element consists of a two-dimensional, eight-phase-step binary grating which acts as a high-throughput nine-fold fan-out optical element with > 80 % diffraction efficiency [11]. This 2D grating, henceforth called a multi-focus grating, was employed in a multifocal, fast 3D microscopy apparatus in which nine cross-sectional planes of an observed specimen, separated by distances ranging from a few hundred nanometers to a couple of microns -depending on the imaging problem at hand-, could be recorded simultaneously on a single imaging plane with diffraction-limited resolution. Reinforcing the idea that a larger number of phase levels is necessary for improved performance, the 80 % efficiency of such 8-level multi-focus grating supersedes a 2-level grating with 67 % diffraction efficiency that has been used previously in the same 3D microscopy setup [5]. The method used to fabricate the multi-focus grating, illustrated in Fig. 1(a), consists of a sequence of three lithography and etch steps with patterns that, overlayed together, result in the complex topography shown in Fig. 1(b).
The remainder of this article is organized as follows. Section 2 briefly introduces the multi-focus grating geometry, design and operating concept. Section 3 introduces the method employed for our theoretical assessment, and presents simulation results for the relevant types of fabrication imperfections. In Section 4, we present experimental measurements of relative power in the different diffraction orders from a fabricated multi-focus grating, taken over a broad wavelength range (100 nm) and with a high spectral resolution through use of a supercontinuum laser source. We show that such measurements can be quite valuable for tracking systematic fabrication errors. It is worth noting that broadband spectral characterization of diffractive optical elements such as shown here has been reported only a few times in the literature [12–14], and either with lower resolution, or over narrower wavelength spans. In particular, broadband, wavelength-dependent characterization of a multi-focus grating was done in [11], albeit with a lower spectral resolution, and limited comparison to theory; here, we show that a sufficiently high spectral resolution over a wide wavelength span can yield clear signatures in the wavelength-dependent relative power of the different diffraction orders that can be verified with a simple theoretical model, and thereby provide valuable information about fabrication imperfections.

2. Multi-focus grating

In this section we briefly introduce the Multi-Focus Gratings demonstrated in [5, 6, 11]. The multi-focus grating consists of a 2D phase grating with spatially-varying unit-cell dimensions. In the multifocal 3D microscopy setup a multi-focus grating is placed after the objective, at a Fourier plane of the microscope, for two purposes. First, as an optimized 2D diffraction grating, it acts as a 9-fold beamsplitter, scattering incident light coming from the objective into the first 9 Bragg diffraction orders in a square pattern. Secondly, at each diffraction order \((m_x, m_y)\), the spatially-varying periodicity of the grating introduces a defocus \(\Delta z(m_x, m_y) = \Delta z \cdot (m_x + N \cdot m_y)\), with \(m_{x,y} \in \{-1, 0, 1\}\) [15]. With this, the different diffraction orders, when focused at a common image plane, simultaneously produce images of objects placed at distances \(\Delta z(m_x, m_y)\) from the objective focus on the optical axis. To provide both of these features, the multi-focus grating is generated by replicating the unit-cell shown Fig. 1(b) across the \(xy\) plane, however with \(x\) and \(y\) cell dimensions varying as \(d_x(x, y) = d \cdot (n \cdot z/\lambda) \sqrt{1 - (x^2 + y^2) / (n \cdot f_{obj})^2}\) and \(d_y = 3 \cdot d_x(x, y)\). Here, \(f_{obj}\) is the objective focal length and \(n\) the immersion medium index.

The original unit cell dimension \(d\) is obtained for a design wavelength \(\lambda\) upon consideration of the spatial separation between the diffracted orders (and ultimately between the focused images for the different focal planes), the total grating aperture and the focal-plane spacing \(\Delta z\) [5, 15].

While the necessary spatial distortion of the unit-cell dimensions follows a known functional form, the unit-cell spatial phase profile is determined via an optimization procedure [3, 6]. In [11], the eight-level binary phase grating shown in Fig. 1(b) was computed to yield a far-field in which the power of an incident beam was split among the first nine diffraction orders in a square array, with overall diffraction efficiency of 89 %. For an ideal grating, each of the eight spots surrounding the zero-order at the center carry 10 % of the total incident power, while the zero-order beam itself carries 9.5 %. This feature is achieved by design to balance image intensity, as the central beam otherwise experiences fewer overall losses in the optical path to the camera.

3. Theoretical assessment

As shown in Fig. 1(a) our process involves a sequence of three aligned optical lithography and anisotropic plasma etching steps. The second and third lithography steps require fine alignment between the etched patterns and the new layer, and fine control of the different etch depths and sidewall angle are essential for superior diffraction performance. Overlay accuracy is limited
by the optical lithography system employed. In particular, the optical projection lithography system available at our laboratory - a state-of-the-art i-line stepper with 5× reduction and maximum resolution of 280 nm - offers a specified 40 nm overlay accuracy. The plasma etching process developed for producing the complex vertical profile of the binary phase grating has an etch rate of 30 nm/min, and allows a depth control accuracy of better than 3 nm (based on a plasma stabilization time of 10 s), with sidewall angles of less than 5°. We now proceed to model the effect of these critical features on the multi-focus grating performance. Further details can be found in [11].

3.1. General theoretical model

We will investigate the diffraction properties of a periodic (undistorted), infinite 2D phase grating illuminated by a plane wave impinging normally at its surface. We assume the electric field to be parallel to the sample surface everywhere, and that it suffers no rotations through the grating, such that we can describe it with a time-harmonic, complex scalar field of the form $E(x, y) = \exp[ik_z(z - z_0)]$, with $z_0 = 0$ set at the first etched surface. As the plane wave traverses the etched phase grating, its phase-front acquires a spatial phase distribution $\Phi(x, y) = 2\pi(n_{\text{glass}} - 1)\delta z(x, y)/\lambda$, where $\lambda$ is the wavelength of light, $n_{\text{glass}}$ the refractive index of the glass and $\delta z(x, y)$ is the local multi-focus grating etch depth, as indicated in Fig. 1(a). Assuming no propagation losses in the glass, the transmitted field at the output is $E_{\text{out}}(x, y) = t_{\text{glass}}^2 E_{\text{in}} \exp[i \Phi(x, y)]$. In the far-field, the diffracted field distribution is simply the 2D Fourier transform of $E(x, y)_{\text{out}}$ [3]. The phase profile $\Phi(x, y)$ is computed by adding together the three subsequent etch depth profiles $z_{1,2,3}(x, y)$: $z(x, y) = \sum_{n=1}^3 d_n \delta(x, y)$, where $\delta(x, y) \in \{0, 1\}$. For a total etch depth $d = \lambda/(n_{\text{glass}} - 1)$, corresponding to a total phase-shift of $2\pi$, we make $d_1 = 4d/7$, $d_2 = 2d/7$ and $d_3 = d/7$. This produces 8 etched levels spaced by $d/7$, or $\pi/7$ (note that $2\pi$ is equivalent to 0 phase). As mentioned above, the phase grating we are interested in, demonstrated in [11], was designed for a wavelength of 515 nm. For a refractive index of $n_{\text{glass}} = 1.469$, obtained from the glass manufacturer, $d = 961$ nm at this wavelength. We take results calculated for an ideal structure with these parameters as the baseline for our comparisons.

In the following subsections, we generate $\Phi(x, y)$ distributions that arise from varying levels of lithography layer misalignment, etch depth and etched sidewall angle variations. We then calculate the corresponding diffraction patterns and evaluate deviations from the ideal case for four figures-of-merit, defined as follows. 1 - Total efficiency decrease: deviation from the nominal 89% total diffraction efficiency into the first 9 diffraction orders; 2 - Zero-order deviation: deviation of the zero-order beam power; 3 - High-order deviation: root-mean-square deviation for the remaining diffraction orders (1 to 8), evaluated as $\sqrt{\sum_{n=1}^8 (P_n - P_{n,\text{ideal}})^2}/8; 4 - Uniformity of the high-order power distribution: standard deviation normalized to the average power of orders 1 to 8.

It is worthwhile pointing out that this type of fabrication tolerance analysis, based on scalar diffraction theory, has been used many times in the literature - see e.g., [16, 17], and is generally appropriate for elements with large features compared to the operating wavelength. As pointed out in [18], however, the presence of small features and asymmetries in the diffractive element (either inherent to the pattern or due fabrication errors) may require more rigorous electromagnetic modeling to yield results with absolute accuracy [18].

3.2. Effect of etch depth

To calculate the effect of variations in each one of the etch steps for the 515 nm design wavelength, we allow $d_1$, $d_2$ and $d_3$ to vary independently within ±40 nm around their respective ideal values, and calculate the corresponding phase distributions $\Phi(x, y)$ for each combination.
Figure 2 shows contour plots for the four figures of merit defined above as functions of the etch depths $d_1$, $d_2$, and $d_3$, taken two at a time. In Fig. 2(a), it is apparent that, for the deviation range considered, the overall efficiency varies by less than 5%. The zero-order diffraction power shown in Fig. 2(b) is very sensitive to small deviations in the first depth, $d_1$, and considerably less so to the second and third etch depths, $d_2$ and $d_3$. The reason for this is that pattern 1 is used to define phase levels 1 to 5, so deviations in $d_1$ affect a greater part of the 7 total etched phase levels. In order for the zero-order power deviation to remain below 10%, a deviation in $|d_1|$ of less than 10 nm is necessary, whereas this requirement is relaxed to beyond 40 nm for both $|d_2|$ and $|d_3|$. Figures 2(c) and (d) show that both the uniformity between the high-order diffracted powers and RMS deviations remain below 10% for the $\pm40$ nm variations covered here. It is also apparent that such figures-of-merit are less sensitive to variations in $d_1$ than in $d_2$ and $d_3$. Most likely, the smaller features defined by patterns 2 and 3 play a stronger role in determining scattering into the high diffraction orders than pattern 1. The sensitivities of the four figures-of-merit as a function of overall etch depth errors are plotted in Fig. 3(a).

3.3. Effect of layer misalignment

To calculate the effect of overlay errors between the three lithography layers, we allow patterns 2 and 3 to be shifted within 250 nm radii of their original positions. Figure 3(b) indicates...
that the total efficiency decrease remains below 10 % for overlay errors of < 150 nm, which
is somewhat relaxed, at least relative to our existing capabilities; however all other figures-
of-merit have stronger requirements, in particular the zero-order power deviation, which is
achievable only for maximum overlay error of < 80 nm.

3.4. Effect of sidewall angle

To study the effects of etched sidewall angle on the performance of our phase grating, we use
a numerical procedure to produce linear phase gradients between the etched and unetched re-
gions of each lithography pattern, corresponding to a particular sidewall slope angle \( \theta_{slope} \). To
do this for a single lithography layer, we produce a series of \( M \) copies of the same (binary) etch
pattern, however with increasingly dilated open regions (i.e., areas on the substrate that are not
protected by photoresist). Each image in the sequence is dilated by a single pixel with respect
to the previous one. This is done by application of a digital dilation filter with a circular flat-
top kernel of appropriate size. Next-neighbor images in the sequence are then subtracted, and
the remaining regions are assigned a uniform phase shift of \( m \cdot dh \), where \( dh = p \cdot \tan(\theta_{slope}) \),
\( m = 1...N \). This image sequence is summed up and added to the the original lithography pattern,
to yield a final phase distribution in which photoresist-protected areas retain the original shape,
however the phase transitions vary linearly between the protected and open areas with the spec-
ified slope. Figure 3(c) indicates that sidewall slopes of above 30\(^\circ\) can lead to overall diffraction
efficiency reductions of above 10 %, and similarly for zero- and high-order diffracted powers.
The zero-order diffracted power displays a maximum at roughly 40\(^\circ\), which is however just
above 10 %. Sidewall control to better than 10\(^\circ\) would keep all figures of merit well within 5 %
uncertainty of the theoretical maximum.

4. Wavelength dependence

4.1. Theoretical Performance

The optimization process leading to the final grating phase distribution does not include any in-
formation about the wavelength of light. As noted above, however, in etched binary phase grat-
ings, the local phase at the grating output surface is given by \( \Phi(x, y) = 2\pi(n_{glass} - 1)\delta z(x, y)/\lambda \),
which can only be optimal at a chosen design wavelength \( \lambda_{design} \). In practice, a maximum etch
depth \( \delta z = d_{total} \) is calculated so that \( \Phi = 2\pi \) at \( \lambda_{design} \). We now evaluate the wavelength-
dependence of our phase grating performance, which had a design wavelength \( \lambda = 515 \text{ nm} \).
The wavelength-dependent variation of the total diffraction efficiency and of the powers carried by the different diffraction orders, normalized to the sum of their power, can be evaluated in Fig. 4. It is apparent that at $\lambda = 515$ nm, the total efficiency is actually not maximal, however, as defined by design, the high diffraction order curves do cross at this optimal point and, in addition, the zero-order power is appropriately lower. Departing from the optimal wavelength, the relative power distribution among the different diffraction orders, and particularly the zero-order power, varies significantly over several nanometers in wavelength. For an overall performance variation of less than 10%, the operating bandwidth is of the order of a few nm. Importantly, however, the diffraction efficiency into the nine main grating orders varies by less than 5% over the entire displayed wavelength span, which means that the nine-fold beam-splitting action is broadband. Thus the same grating can still be utilized for wavelengths very far from the designed wavelength, albeit with sub-optimal performance.

![Fig. 4. Calculated diffraction efficiencies into the first nine orders as a function of wavelength for the ideal multi-focus grating design ($\lambda = 515$ nm). Top: sum of the nine orders; Bottom: individual orders.](image)

4.2. Experimental characterization

We now show experimental measurements of the diffraction performance from a multi-focus grating produced at an initial fabrication round. Such a measurement was carried out to determine potential discrepancies with the theoretically-expected results, which could be traced out to systematic fabrication errors. The grating was fabricated through the process outlined above and in [11], on a 500 $\mu$m-thick fused silica substrate. To characterize the sample optically, we used a supercontinuum laser source with a broadband spectrum which covered at least the entire range of wavelengths between 470 nm and 560 nm. The supercontinuum laser light was passed
through a monochromator, then coupled into an optical fiber with a 600 nm single-mode cutoff wavelength, which acted as a spatial filter. The monochromator had manually adjustable wavelength selection with a specified wavelength accuracy of ±0.2 %, and specified bandwidth of 1 nm. With the broad supercontinuum laser spectrum (ranging from ≈ 400 nm to ≈ 1000 nm), and its high spatial coherence, this apparatus acted as a spatially coherent, extremely broadband, high resolution tunable light source. Light from the optical fiber was launched into free-space with a collimator, then focused onto the grating at normal incidence, with a 100 mm singlet lens. The illuminating spot size at the multi-focus grating was of ≈ 2 mm, which means that it sampled only a small portion of the ≈ 1 cm diameter of the fabricated grating. A complementary metal-oxide semiconductor (CMOS) camera was placed immediately after the sample to record the transmitted diffraction pattern. A schematic of the measurement setup is shown in Fig. 5.

Fig. 5. Experimental setup used for measuring diffraction orders of the multi-focus grating over a wide wavelength range. MFG: multi-focus grating.

Raw RGB images, taken without gamma correction, were converted to grayscale intensities by calculating the luminance $Y$ through the standard NTSC conversion $Y = 0.2989 \times R + 0.5870 \times G + 0.1140 \times B$ ($R$, $G$, $B$ here are the intensities of the red, green and blue components). An example image is shown in Fig. 6(a). Also shown are the powers carried in each diffraction order, normalized by the sum of the powers. To obtain these values, we proceeded as follows. First, a sequence of 21 images was taken of the diffraction pattern. Background images were also taken by covering the laser source output. From these, we created background-subtracted, averaged images of the diffraction pattern. Next, we defined a grid of contiguous and equally sized square regions, or fields, centered at the diffraction spots. Within each such fields, we integrated the pixel intensities over a sequence of square subregions of increasing areas, centered at the field center, as illustrated in the inset of Fig. 6(b). We thus produced, for each field, an array of integrated intensity with respect to integration area, which captured not only the intensity of the main diffraction spot, but also the intensity of the immediately surrounding background [red line in Fig. 6(b)]. The origin of this background was undetermined and constituted a significant source of uncertainty in our measurement. Assuming that, for areas larger than the central diffraction spot within each field, a constant intensity background dominated the image intensity, we expected that the integrated intensity would show a linear dependence on the integration area. As such, we fit the last ten samples of our integrated intensity array, in each field, with a linear function of the integration area [black dashed curve in Fig. 6(b)], and subtracted the fitted curve from the original array. This gave us a sequence of background-subtracted integrated intensities, plotted in blue in Fig. 6(b). We then took the mean of this and the unsubtracted intensities integrated over the entire field to estimate the power in the corresponding diffraction order. The magnitude of difference between the two was taken as our measurement uncertainty. Figure 6(a) shows an example result of such calculation, where the all powers and uncertainties were normalized to the sum of the mean integrated
intensities. To verify the linearity of the power extracted from the camera images through this procedure, with respect to the actual optical power of the measured beams, we performed a calibration measurement with results displayed in Fig. 6(c). Here, the linearly-polarized output of a single-wavelength, continuous-wave diode-pumped solid-state laser fixed at 532 nm was passed through a half-wave plate and a polarizer, for power control, and then through a 50:50 cube beam splitter. The CMOS camera was placed at one of the beamsplitter outputs, while a broad-area photodetector was placed at the other output, so that beam power could be measured simultaneously with the camera images. As shown in Fig. 6(c), the extracted integrated intensities varies linearly with input beam power. We point out that this measurement was performed for beam intensity levels comparable to those used in the multi-focus grating characterization.

Fig. 6. (a) Experimental multi-focus grating diffraction pattern at $\lambda = 550$ nm, recorded with a CMOS camera. Nine orders, labeled $(m, n)$, $m, n = -1, 0, 1$, are shown. Yellow numbers are the intensity in each diffraction order, normalized to the sum of all nine intensities. Errors are of one standard deviation, as explained in the main text. (b) Integrated intensity for one diffraction order (shown in the inset) as a function of integration area. Blue: Background-corrected; red: uncorrected; dashed: linear fit to last ten samples of red curve. The telescoping integration area used is illustrated in the inset. (c) Calibration of the diffraction order power measurement, showing integrated intensity for a single, 532 nm laser beam spot as a function of beam power. Circles: experimental data; continuous line: linear fit.

For the multi-focus grating characterization, the procedure outlined above was repeated for a range of wavelengths, and the results are displayed in Fig. 7. It is important to point out that the measured values do not correspond to the diffraction efficiency in each order, since the integrated intensities are normalized by the sum of the intensities, rather than the total incident power. For that, an additional measurement would have had to be performed, of the incident beams before the multi-focus grating, which would add further complexity and experimental uncertainty to the procedure. Nonetheless, the present data still yields very useful information regarding our grating. The experimental data in Fig. 7 shows that the zero-order diffraction intensity is consistently lower than the theoretically expected one for wavelengths longer than 490 nm, which, together with the fact that the powers for all the orders only became comparable close to that wavelength, suggest that the center wavelength for the grating is blue-shifted; or, alternatively, that the etched gratings are too shallow for an operating wavelength of 515 nm. To verify this, we used an optical profilometer to determine the spacings between etched levels on the fabricated grating. These measurements pointed to a maximum discrepancy of less than 20 nm from the ideal values, which could not account for the observed blue shift. We then ran a series of diffraction pattern calculations with level spacings taken from the optical profilometer measurements, and adjusted the refractive index until we obtained a reasonably good agree-
ment with the data, shown in Fig. 7. The best-fit refractive index was $n_{\text{glass}} = 1.458$, 0.75 % lower than that considered in the original design. Importantly, this small difference in refractive index actually results in a significant difference, of 2.3 %, in the local phase $\Phi(x, y)$, which is proportional to the index difference ($n_{\text{glass}} - 1$). With this index contrast and the ideal etched level spacing, the operating wavelength becomes 503 nm, almost 10 nm blue-shifted from the original. The excellent agreement between theory and experiment, particularly for the $(0, 0)$ and $(0, \pm 1)$ orders highlighted in Fig. 7, suggests that the refractive index used in the preliminary design indeed led to shallow gratings and the observed wavelength shift.

Fig. 7. Intensity of the nine diffraction orders, normalized by the sum of the intensities, as a function of wavelength, for a non-ideal multi-focus grating. Continuous lines: simulation, assuming grating steps measured from the fabricated sample. Symbols: measured quantities from the same fabricated multi-focus grating. Matching colors correspond to the same diffraction orders in calculation and experiment (note that some of the simulated curves are coincident throughout, so only five curves effectively appear on the graph). Intensity error bars are for one standard deviation, as explained in the main text. Horizontal error bars correspond to a 20 % manufacturer-specified monochromator wavelength uncertainty.

5. Conclusion

In summary, we have performed a comprehensive theoretical assessment of fabrication tolerances for a 2D eight-level binary phase grating that is the central element of a multi-focal plane 3D microscopy apparatus. Our analysis shows that small fabrication imperfections can lead to degradation in the diffraction efficiency, uniformity and, importantly, the power in the zeroth-order term, which is of particular importance in the 3D multifocus microscopy technique described in Refs. [5, 6, 11]. The most challenging tolerance to meet is that for overlay accuracy between the layers. A layer-to-layer misalignment of less than 80 nm is necessary for overall performance degradation below 10 %. Etch depth needs to be controlled to better than 10 nm, primarily due to degradation of the zero-order beam intensity; all other figures-of-merit
are not strongly affected at least up to 40 nm variations in etch depth. These stringent requirements are nonetheless achievable with current state-of-the-art projection lithography systems. Lastly, etched sidewall angles below 30° are necessary for overall performance degradation below 10%.

We have also developed a measurement of fabricated multi-focus grating diffraction patterns, which allowed us to uncover a systematic fabrication error in a clear and straightforward way. Making use of widely tunable light source based on a supercontinuum laser, we were able to determine the evolution of the relative powers of the nine diffraction orders produced by a fabricated multi-focus grating over an optical bandwidth of 100 nanometers (a much wider bandwidth would be possible). Over such a broad wavelength range, the variation of relative intensities between the diffraction orders was significant enough to provide a clear signature that could be replicated by a simple theoretical model. We thus believe that this type of measurement can be of great value for characterizing binary optical elements.

Appendix: Finite-difference time-domain simulation verification

In [18], it was shown that rigorous electromagnetic simulations may be necessary to predict the performance of diffractive optical elements with very small features compared to the wavelength, either by design or due to fabrication errors. To verify whether the scalar model used here produced reasonable results for a sensitivity analysis of our multi-focus grating, we performed finite-difference time-domain (FDTD) simulations of the diffractive element illuminated by a plane-wave. The FDTD method solves the full-vector Maxwell’s equation in time-domain, is commonly used to simulate optical elements with sub-wavelength features, and has been used in the past to model similar types of diffraction optics as here [19]. Simulation results for the original grating, and one in which two layers are misaligned by an amount in both the x and y directions are provided in Fig. 8 below, for Δ = 143 nm and Δ = 238 nm. For each case, the diffraction efficiency and the relative power in each of the orders normalized to the total power in the nine orders, all as a function of wavelength, are shown.

![Finite-difference time-domain calculated diffraction efficiencies into the first nine orders as a function of wavelength, for multi-focus gratings with layer-to-layer deviations Δ = 0, Δ = 143 nm and Δ = 238 nm. Top: sum of the nine orders; Bottom: intensity of the nine diffraction orders, normalized by the sum of the intensities. The dashed line marks the design wavelength.](image)

The first thing to note is that the evolution of the curves with respect to wavelength is very similar to observed in Fig. 4, obtained with the scalar model (note that the scalar model does not take transmission loss at the glass-air interface, which accounts for the overall higher diffraction
efficiency in that case). We point out that the original pattern already has features that are considerably smaller than the wavelength, and so the observed discrepancies between the FDTD and the scalar model are not unexpected, according to [18]. Because the focus of our paper is on a sensitivity analysis, however, we use the FDTD simulation for the original grating as a baseline.

At the design wavelength, respectively for misalignments $\Delta = 143$ nm and $\Delta = 148$ nm, the diffraction efficiency into the 9 main orders decreases by 3 % and 6 % and the zero-order power deviation varies by 4 % and 11 %, with respect to the baseline ($\Delta = 0$). The degree of non-uniformity of the high-order powers is already 10 % for the grating without layer misalignment, and reaches 12 % and 17 % for $\Delta = 143$ nm and $\Delta = 148$ nm. This is the most significant difference we see between the scalar and full-wave results. These results show that, at least for the particular diffractive element studied here, the scalar model provides reasonable guidance for fabrication tolerances.

**Acknowledgments**

We thank Sara Abrahamsson from Rockefeller University, New York, NY and Jan Wisniewski from the HHMI Janelia Research Campus, Ashburn, VA, for useful discussions.