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Authors

Yashchuk, Valeriy V

Takacs, Peter Z

Lacey, Ian

et al.

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Improvements in optical metrology for high-performance variable-line-spacing x-ray gratings

Valeriy V. Yashchuk^a, Peter Z. Takacs^b, Ian Lacey^a, Keiko Munechika^c, Kaito Yamada^c, and Simon Rochester^d

^aAdvanced Light Source, LBNL, 1 Cyclotron Road, Berkeley, CA 94720, USA; ^bSurface Metrology Solutions, LLC, 19 S 1st St, Unit B901, Minneapolis, MN 55401 USA; ^cHighRI Optics, Inc., 5401 Broadway Terr, St. 304, Oakland, CA 94618, USA; ^dRochester Scientific, LLC, 2041 Tapscott Avenue, El Cerrito, CA 94530, USA

Abstract

We discuss a project to develop a precision metrology system for variable-line-spacing x-ray gratings using interferometric microscopes. We are developing test standards and calibration techniques to measure and correct for geometrical distortion and blur, and data processing techniques to combine multiple measurements and measure line spacing with high accuracy.

1 Introduction

Variable-line-spacing (VLS) gratings are employed as the main elements of many x-ray spectrometers and monochromators.¹ Spectrometers with VLS gratings can disperse the spectrum in a focal plane almost perpendicular to the diffracted beams and allow formation of stigmatic spectral images. Steady improvements to these instruments have tightened the requirements for the groove frequency, shape, and phase coherence of the gratings. Next-generation gratings are under development for the ALS (Advanced Light Source) and ALS-U beamlines at LBNL, in particular, in the DOE Basic Energy Sciences (BES) funded project “21st Century Methods for Making Gratings” at ALS.

To enable fabrication of these optics at reasonable cost, advanced surface metrology with both high accuracy and high measurement rate must be available to integrate into modern deterministic surface figuring/patterning processes. After fabrication, additional surface metrology techniques are used at the x-ray facilities to ensure that the quality of the optical surface is adequate to the specifications of the beamline optical system and end-station. Confidence in the beamline optical design and fabrication specifications critically depends on the availability of trustworthy before-fabrication models of the optics, based on metrology data obtained with existing optics. Under- and over-specifications are both undesirable, the former because of the risk of beamline performance degradation, the latter due to the unnecessary cost increase.

Unfortunately, existing metrology tools and data acquisition and processing methods are insufficient to meet today's challenges. The available metrology instrumentation in use at the DOE BES light-source facilities, as well as in the U.S. optical fabrication industry, including traditional long trace profilometry, deflectometry, interferometry, and microscopy, have essentially reached the limits set by available optical and mechanical materials and components, as well as by the nature of the physical processes used for measurement.^{2,3} For example, spurious effects due to light diffraction and interference and the imperfection of optical elements contribute to systematic error and limit lateral resolution. To decrease the contribution of systematic errors, multiply repeated measurements designed to anti-correlate the errors have to be performed,⁴⁻⁶ leading to low measurement rates, usually unacceptable in the optical fabrication industry.

For example, the conventional technique⁸⁻¹⁰ for characterization of the groove density distribution of VLS gratings is based on measurement of the diffraction angle with a long trace profiler (LTP) in the Littrow configuration. In many cases, LTP metrology is capable of measuring groove density distributions with the required accuracy, but, due to low spatial resolution, fails to measure groove phase coherence, which

determines the beamline spectral resolution achievable with the grating. Moreover, when applied to gratings with rapid variation of the groove density, the LTP-based technique has fundamental limitations in both local accuracy and dynamic range (the ratio of largest to smallest measurement scales). First, the steep variation of the groove density leads to a large variation of the optical path within the diffracted LTP sample light beam, causing a strong interference effect in the beam intensity distribution recorded with the LTP detector and making it practically impossible to measure the local diffraction angle with the required accuracy. This problem, illustrated in Figure 1, was encountered in the LTP-II measurements at the ALS X-Ray Optics Laboratory (XROL) of the VLS grating for the ALS AMBER beamline.⁷ Second, the overall variation of the groove density can significantly surpass the angular dynamic range of the LTP (typically about 10 mrad). For example, in the above measurement, the LTP could perform a single scan only over a 12-mm region out of the total length of 80 mm. Therefore, to thoroughly characterize the grating, one would need to stitch together at least 8 scans (assuming 2 mm overlap), performed with different pitch tilts of the grating. Such stitching requires high-precision absolute measurements of the incidence and diffraction angles for each point of a scan, which is extremely difficult because of the uncertainty in the LTP angular coordinate system reference.

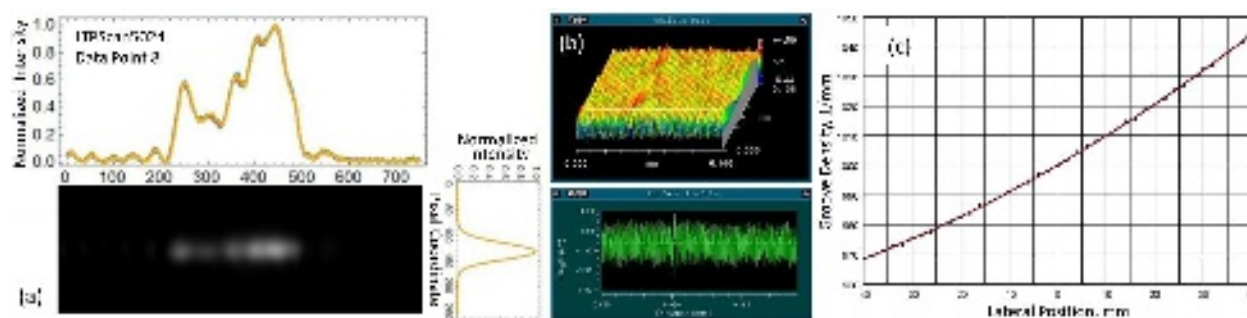


Figure 1. (a) Intensity distribution of the diffracted light beam recorded with the LTP-II CCD detector while measuring the AMBER VLS grating. The distribution is strongly affected by the inter-beam interference due to the strong variation of the groove density. (b) Surface profile of the same grating measured with the Zygo NewView-7300 microscope. (c) Groove density distribution extracted from the measurement. (For more details see Ref. 7)

We are developing a high-accuracy microstitching interferometry (MSI) system, based on commercially available interferometric microscopes, for direct measurement of surface topography over the entire clear aperture of a VLS grating. We plan to achieve higher accuracy and dynamic range than is currently available, without major modifications to the instrument itself, by leveraging calibration and data processing techniques under development by our collaboration: procedures for combining interferometric measurements to increase both image size and resolution, as well as test samples, measurement protocols, algorithms, and software to characterize and correct for the instrument response, reducing blurring, geometrical distortion, and other sources of systematic error.

The goal is to establish MSI metrology capable of high-accuracy (on the level of ~ 10 nm or below) measurement of groove position over the entire clear aperture of the grating (up to a length of 0.5 m). This will enable not only accurate predictions of diffracted x-ray beam quality (determined by the groove density distribution), but also of the grating energy resolution (determined by the groove spatial coherence).

Although development will take place around the NewView-9000, our system need not be restricted to use with this particular interferometric microscope. In fact, the techniques we are developing are generalizable to a wide range of metrology tools aside from interferometric microscopes.

We plan to significantly improve the performance of the metrology on the instrumentation used for characterization of x-ray optics, through development of data acquisition methods,^{4–6} calibration techniques^{11–19} and data analysis and correction based calibration,^{20–22} and by integrating these technologies into the metrology workflow.

2 Grating frequency estimation

A surface profile measurement of an x-ray grating from an instrument such as the Zygo NewViewTM-9000 interferometric microscope (Figure 2a) can be analyzed to estimate the local grating frequency. We are developing several different techniques for such an analysis, including a method using the power spectrogram of the measurement, a technique first suggested and demonstrated at the ALS XROL.²³ We discuss this analysis and our approaches to enhancing it in this section.

We are currently developing three techniques for VLS grating local frequency estimation—the zero-crossing method, the power spectrogram method, and the fitting method. We apply these techniques both to the one-dimensional transverse-mean profile as well as the two-dimensional profile.

In the zero-crossing method, the positions of the zero-crossings of the surface profile are located using linear interpolation, and the local grating frequency is found assuming that each grating period contains two zero crossings. In the power spectrogram method, the power spectrogram is found as the absolute square of a sliding-window Fourier transform of the surface profile (Figure 2d). The frequency peak of the spectrogram at each position along the grating is an estimate of the local grating frequency. In the fitting method, the surface profile is fit using a harmonic series model with a polynomially varying frequency (Figure 2e). The local frequency estimates obtained for each of the three methods applied to the transverse-mean grating profile are shown in Figure 2f. The three estimates agree, although with varying degrees of smoothness. The smoothness of the power spectrogram estimate is adjustable, depending on the width of the sliding window used.

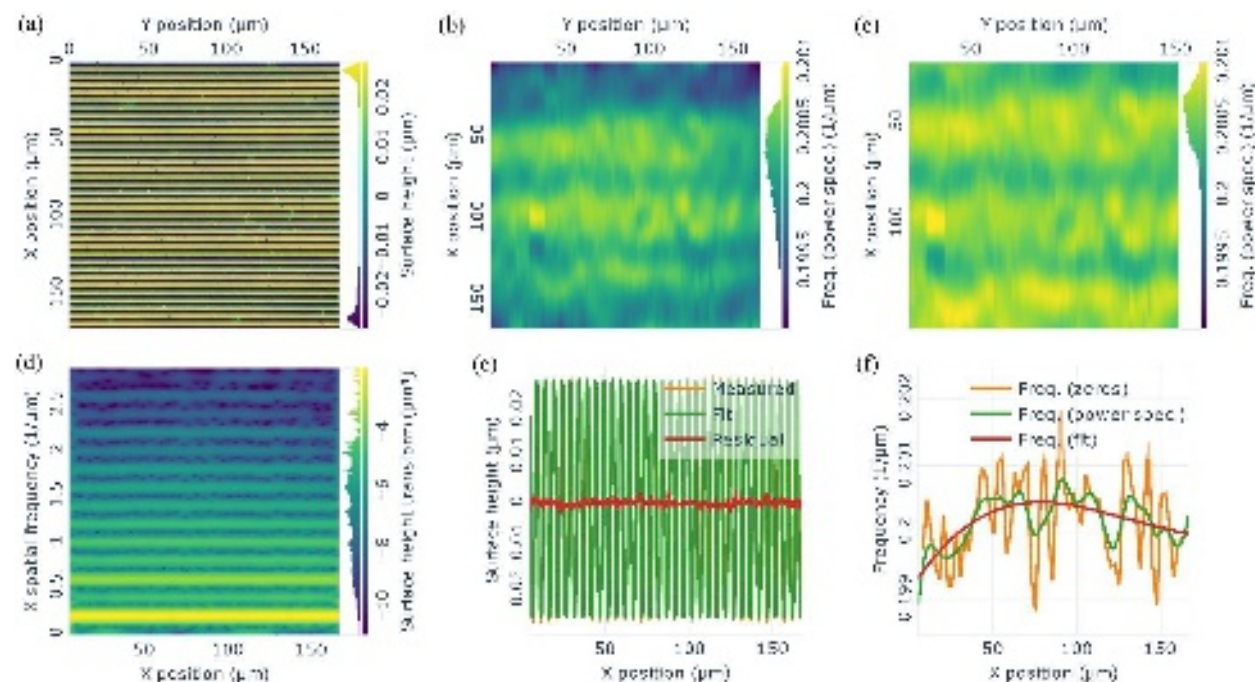


Figure 2. Grating frequency estimation for a nominally constant-frequency grating. (a) Surface profile measurement; (b) 2D frequency estimate from power spectrogram before and (c) after geometrical distortion correction; (d) 1D mean power spectrogram; (e) fit to 1D mean profile; (f) 1D local frequency estimate from zero-crossing, power spectrogram, and fitting methods.

We can also perform a 2D local frequency estimate by applying the 1D techniques to the measurements at each position transverse to the grating axis (i.e., each column of pixels). A 2D local frequency estimate using the power spectrogram method is shown in Figure 2b. Note that, although this is nominally a constant-frequency grating, the apparent frequency falls near the edges of Figure 2b, particularly the top and bottom edges, and at the beginning and end of Figure 2f. This is at least partly due to geometrical distortion, discussed in the next section.

3 Calibration and correction of geometrical distortion

We have shown²⁴ that lens distortion in the surface profile measurement can cause significant errors in grating frequency estimation and that these errors can be reduced via distortion calibration with a standard target.

Distortion calibration is done by finding a best-fit pinhole camera model with radial distortion term that projects the corner features of the design image of a target to the corresponding features in a measurement of that target. Traditionally a checkerboard-type target is used; we use both checkerboard and so-called uniformly redundant array (URA) targets, discussed in Sec. 6.

The corner features in the measurement are located in a two stage process. First, the measurement is registered with the design pattern by taking the radially averaged power spectral density to find the symmetry axis of the measurement and then the linear averages of the profile along and transverse to the symmetry axis to extract the grid pattern. This registration results in an initial camera model that indicates the approximate positions of the projected corner features. In the second stage, the corner positions are refined to subpixel accuracy (Figure 3) using a method based on a localized Radon transform performed using box filters.²⁵

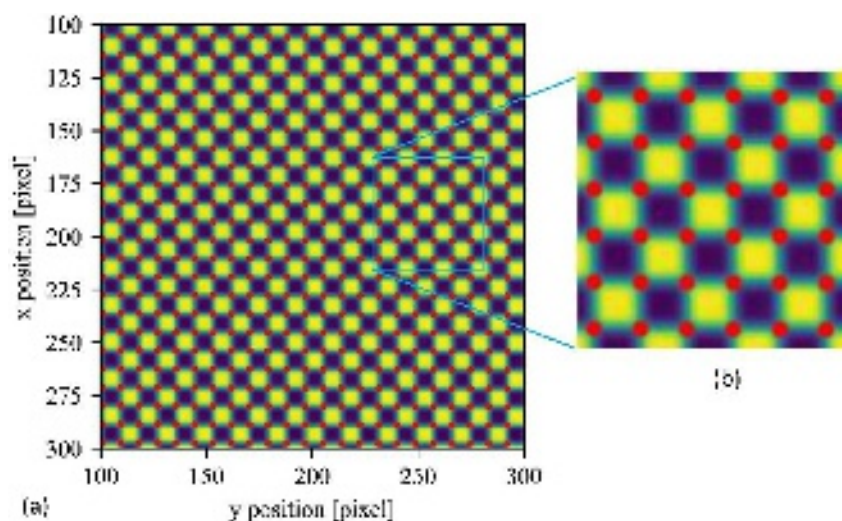


Figure 3. (a) A 200 x 200-pixel section of a 1000 x 1000-pixel image of the 1.5 μm checkerboard; (b) red dots indicate corners found by the algorithm described in the text.

After the corner features are located to within a fraction of a pixel, a best-fit camera model, including a lowest-order radial distortion term, is obtained. Figure 4 shows the residual distances between the measured checkerboard corners and the best-fit projection of the ideal checkerboard corners. When the distortion effect is omitted from the projection model (Figure 4a), the displacement exhibits r^3 dependence (characteristic of barrel distortion) with residual distance of up to two pixels at the image corners. Accounting in the projection model for the lowest-order radial camera distortion, the measured and ideal checkerboard patterns match well (Figure 4b). Thus, the observed lens distortion is well

described by the lowest-order radial distortion term, with the residual distance between projected and measured corners less than 0.05 of a pixel. This also gives a high-accuracy estimate of the real-world size corresponding to each pixel.

The extracted distortion calibration can be used to correct a sample measurement by applying the inverse coordinate transformation and resampling using bilinear interpolation. Such a correction has been performed for the measurement of a constant-frequency grating; as shown in Figure 2c, this greatly reduces the spurious large-scale frequency variation in the measurement.

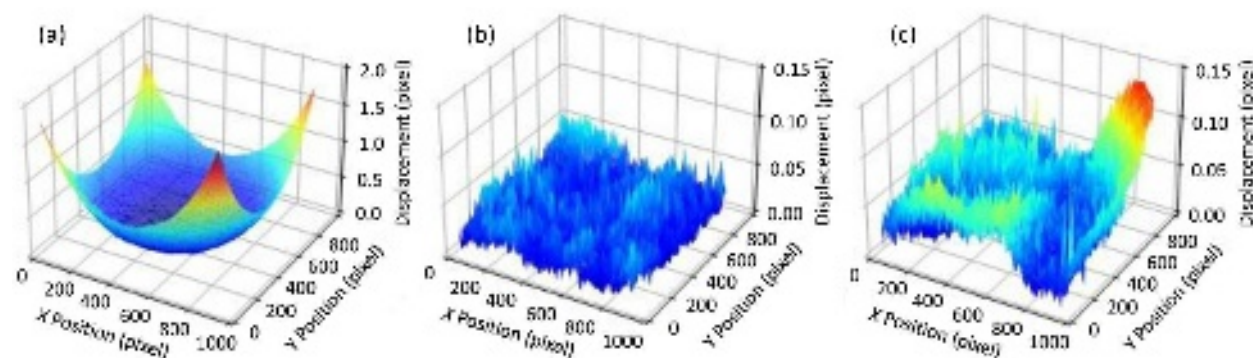


Figure 4. Displacement (in pixels) between the checkerboard corners found from the image and those of an ideal checkerboard projected onto the image, rotated and translated for the best fit. (a) Projection neglects camera distortion; (b) projection accounts for lowest-order radial camera distortion. (c) Displacement (in pixels) between the checkerboard corners found from the resampled undistorted image and those of an ideal checkerboard projected onto the image, rotating and translating for the best fit. Note the difference in vertical scale.

4 ITF measurement and deconvolution

The surface profile measurement of a grating is also subject to the optical blurring characteristic of the instrument and the specific measurement arrangement. The effects of blurring can be mitigated by measuring and deconvolving the instrumental transfer function (ITF) of the microscope. Since high-frequency noise, as well as signal, is amplified in this procedure, it will not improve the accuracy of grating frequency estimation. However, it will significantly improve the characterization of the groove shape. We have pioneered the technique of microscope ITF calibration using the measurement of a binary pseudo-random array (BPRA) standard.^{22,26–28} This technique can be applied to a broad spectrum of metrology tools; we have demonstrated its effectiveness for electron, x-ray, and visible-light microscopes,^{14,15,17,18,22,29} as well as for large-aperture Fizeau interferometers.^{16,30,31}

Figure 5 is a screenshot showing processing of a measurement of the highly randomized array (HRA) pattern with elementary size 81 nm fabricated on a 1-in diameter super-polished Si substrate. The HRA pattern is a white-noise-like binary array, and as such it has a flat PSD. However, the measured PSD (blue curves in the lower right corner of Figure 5) rolls off at higher frequencies due to the ITF of the microscope. Indeed, the observed PSD is a direct measurement of the ITF (plus experimental noise)—this is the primary benefit of using the HRA test standard. In the case depicted in Figure 5, the spatial resolution is significantly lower than if it were limited by the effective pixel size of about 172 nm. The observed resolution corresponds to the Abbe diffraction limit of ~520 nm for the light wavelength of 570 nm and numerical aperture (NA) of 0.55 of the 50× objective used in the present Zygo NewView-9000 interferometric microscope measurements.³²

Using the measured PSD, the best-fit parameters for an analytical model of the ITF can be extracted. (Development of ITF models for the relevant instruments is an objective for our project.³²) With the known ITF for a particular microscope configuration, high-frequency information can be corrected via regularized deconvolution in any subsequent measurement made using that configuration. Our software,

depicted in Figure 5, can deconvolve the measured data using a specified ITF extracted from the BPRA measurement. The deconvolved BPRA height profile measurement is shown in the upper right corner of Figure 5. Corresponding 1D PSDs appear as the orange curves at lower right. We see that deconvolution allows recovering the PSD spectrum at spatial frequencies above $\sim 1.2 \mu\text{m}^{-1}$ by a factor of ~ 10 and even more at higher frequencies. It can be concluded that the upper limit of the groove density range achievable in the measurements with the NewView-9000 microscope is $\sim 1,900$ lines/mm, which is consistent with the Abbe limit of ~ 520 nm derived above.

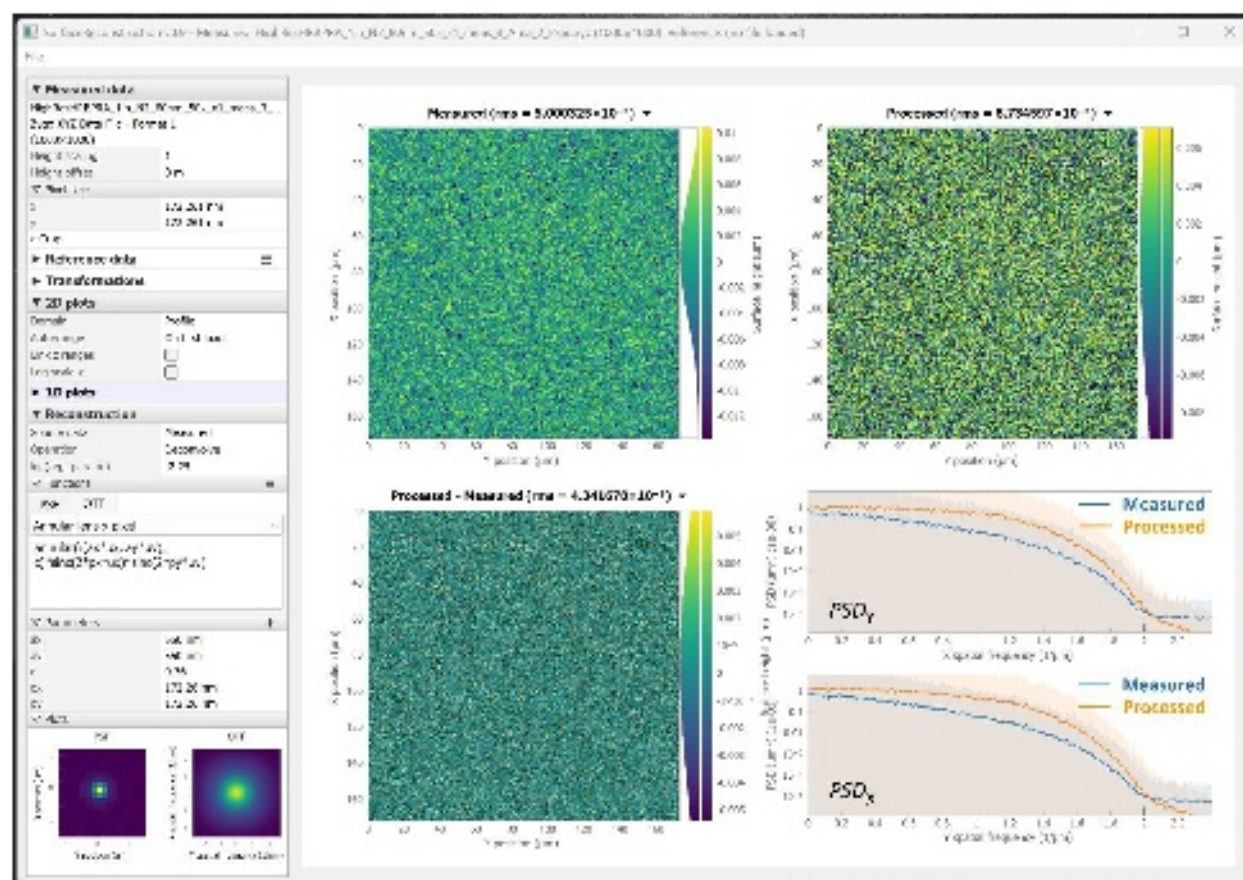


Figure 5. A screenshot of our software for ITF calibration of metrology profilometers and ITF-based deconvolution of the measured data. The data shown was recorded with an HRA standard with elementary size 81 nm using the Zygo NewView-9000 interferometric microscope equipped with $50\times$ objective and $1\times$ zoom lens. The 1D PSD distributions of the measured (blue lines) and deconvolved (orange lines) profiles are shown in the bottom right part of the screenshot.

Figure 6 shows the result of applying the reconstruction (deconvolution) procedure to the measurement of the aBeam “Beameter” chirped test pattern, similar to the VLS gratings relevant to this work. In this case, the processed data are the result of reconstruction based on ITF calibration using a HRA target in Figure 5. From the difference between amplitudes of the horizontal (X) and vertical (Y) cross-sections of the measured and reconstructed profiles in Figure 6, we see that a significant amount of the high-frequency detail of the test pattern can be recovered based on the developed calibration and deconvolution reconstruction technique.

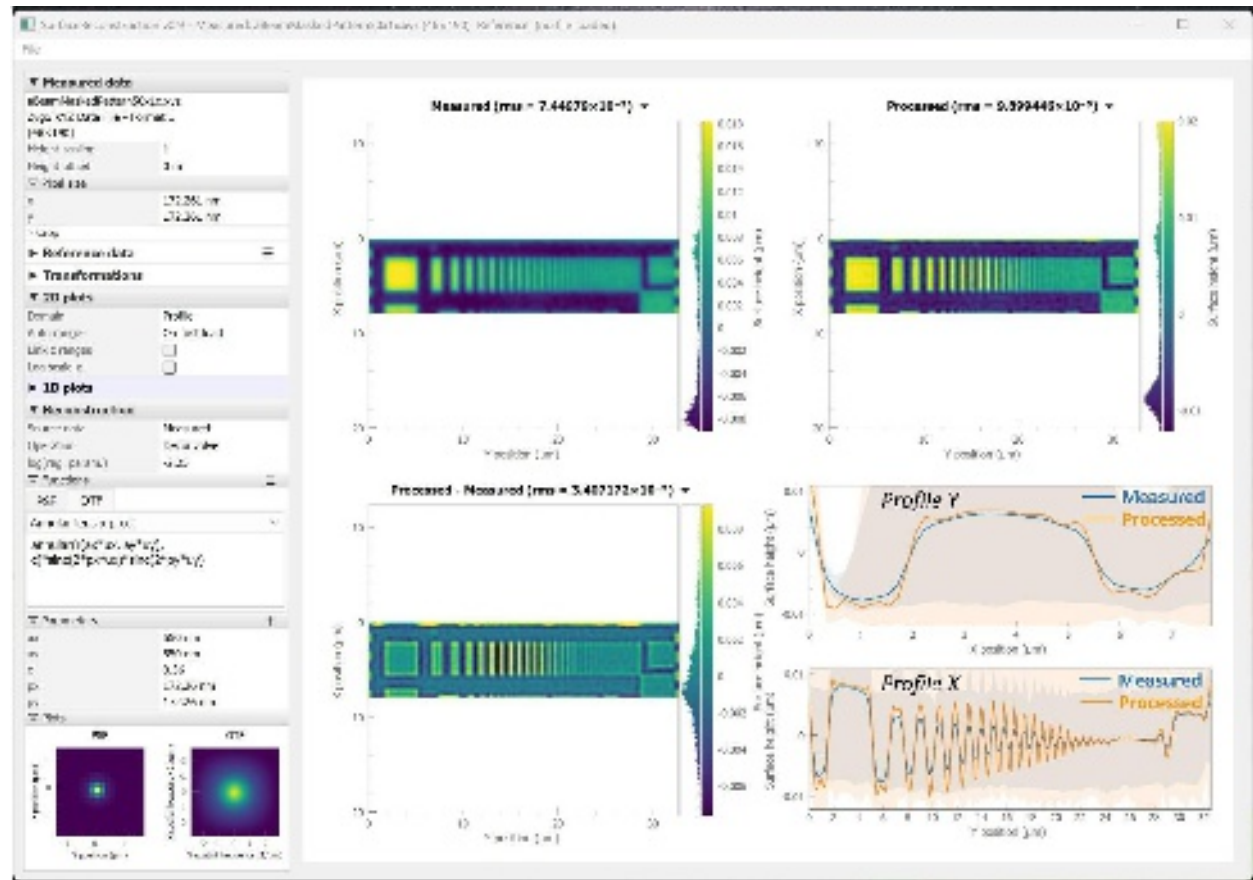


Figure 6. A screenshot of our software for ITF calibration of metrology profilometers and ITF-based deconvolution of the measured data. The measured data shown was recorded with the aBeam “Beamer” test pattern using the Zygo NewView-9000 interferometric microscope in the same arrangement as in the calibration measurements in Figure 5. The processed data are the result of reconstruction based on ITF calibration using the HRA target (Figure 5). The differences between the amplitudes of the horizontal (X) and vertical (Y) cross-sections of the measured and reconstructed profiles depict the efficacy of the reconstruction.

5 Image stitching

To increase the effective dynamic range of a metrology instrument, measurements can be made at different positions on the optic, and the resulting data sets can be stitched together. Multiple partially overlapping measurements (with 50–70% overlap) can be used to provide aggregate measurements over a large area.

Software supplied by instrument manufacturers (such as Zygo Mx) is capable of performing such image stitching. However, because this software does not take into account effects such as geometrical distortion the results can have unacceptable errors (Figure 7).

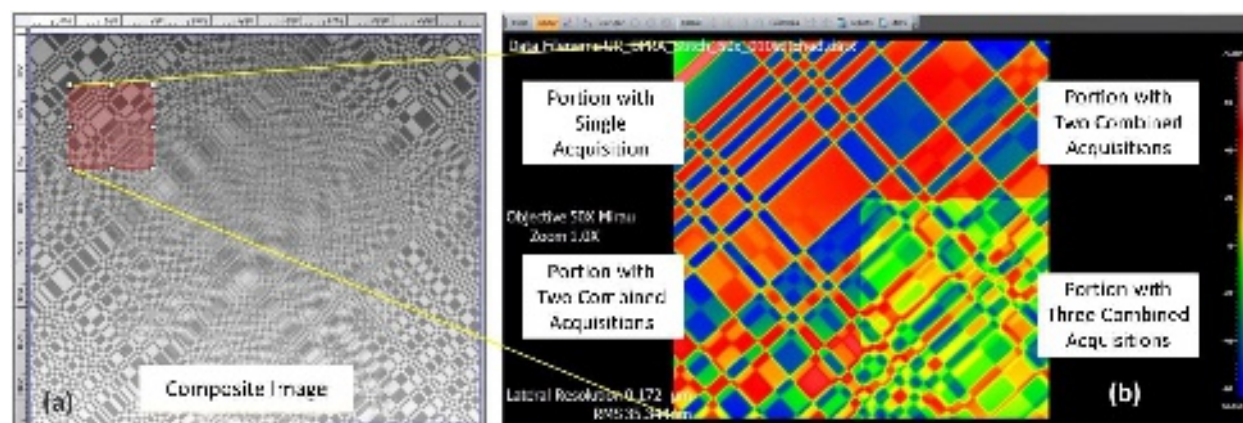


Figure 7. The result of application of the Zygo Mx software stitching procedure to measurements of a URA sample using the NewView-9000. (a) The 3×3 stitched area of the URA sample; (b) magnified region. The observed mismatch is due to the limited performance of the Mx software stitching procedure.

Related techniques are used in the industry-leading MSI/RADSI (microstitching interferometry/relative-angle determinable stitching interferometry) metrology system, recently developed at the Ultra-Precision Machining Laboratory at Osaka University (Japan).^{33–37} However, recent evidence^{20,21,38} has shown that this technology is subject to significant uncharacterized quasi-periodic systematic errors, such as are characteristic of practically all x-ray optics fabrication with deterministic polishing techniques.

We will apply the geometrical distortion and ITF calibration techniques discussed above to correct such errors.

6 Development of test standards

We have designed and fabricated custom test standards and artifacts to measure the ITF and geometrical (lens) distortion. For the ITF calibration we have created BPRA standards with two types of patterns: so-called uniformly redundant arrays (URA)^{39,40} and highly randomized arrays (HRA).³¹ The fundamental (smallest) feature size for these patterns is between 1.5 nm–750 μm , depending on the application.

Figure 8a shows an example of the URA pattern used in this work. This is one of the eight BPRA patterns included in our 2-in diameter BPRA standard depicted in Figure 8b and described in detail elsewhere.^{26,27} There are four URA patterns (fundamental sizes of 2.5 μm , 1.2 μm , 800 nm, and 400 nm), and four HRA patterns (2.501 μm , 1.201 μm , 801 nm, and 401 nm). In this sample, the etched depth of the patterns is about 95 nm. For higher-resolution calibration of optical surface profilometers, we have also fabricated a standard on 1-in diameter super-polished silicon substrate with three HRA patterns (fundamental sizes 241 nm, 161 nm, and 81 nm) – Figure 8c. The etched depth of the HRA patterns is about 40 nm.³² Figure 8d shows a scanning electron microscope image of the 81-nm HRA pattern.

We have also designed and fabricated traditional checkerboard test artifacts.^{22,26} The checkerboard sample has two patterns with fundamental sizes 3.0 μm and 1.5 μm , respectively, etched to a depth of about 15 nm on 1-in diameter super-polished silicon substrate.

The HRA patterns are optimized for ITF calibration, while the checkerboard patterns are optimized for geometrical distortion calibration. However, the URA patterns, which combine the pseudo-random aspect of the HRA patterns and the precisely locatable corner features of the checkerboard patterns, can be used for both types of calibration. We are also developing a “universal” URA pattern that can be used for simultaneous ITF and distortion calibration with a single measurement. This will require a fundamental feature size below the effective pixel size of the instrument, for accurate ITF calibration at high frequencies, and also a significant fraction of larger scale rectangular features, for distortion calibration.

The image registration step in the geometrical distortion calibration algorithm may need to be adjusted to account for the unresolved features in the measurement of such a sample.

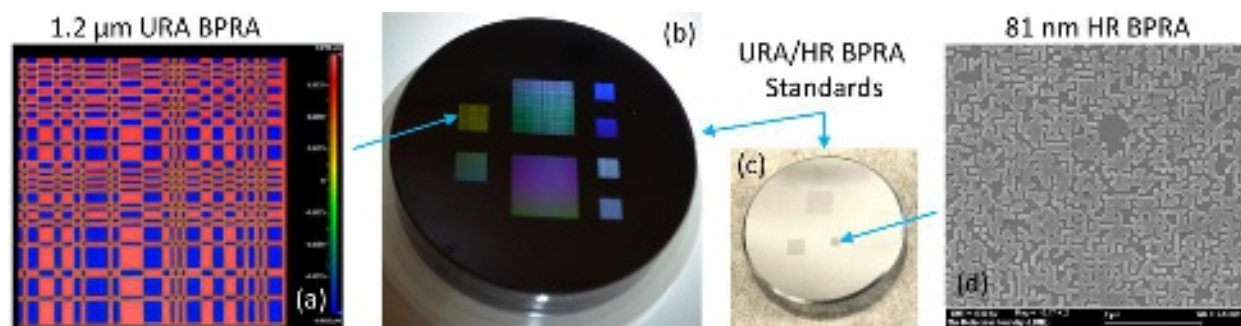


Figure 8. (a) The URA pattern with elementary size of 1.2 μm as measured with the interferometric microscope equipped with 50 $\times$ objective at 1 $\times$ zoom. (b) The 2-in diameter BPRA standard with four URA patterns (fundamental sizes of 2.5 μm , 1.2 μm , 800 nm, and 400 nm), and four HRA patterns (2.501 μm , 1.201 μm , 801 nm, and 401 nm). (c) The 1-in diameter high-resolution calibration standard with three HRA patterns (fundamental sizes 241 nm, 161 nm, and 81 nm).^{26,27} (d) A scanning electron microscope image of the 81-nm HR BPRA pattern.

Conclusions

We have outlined an ongoing project to advance metrology for variable-line-spacing x-ray gratings. BPRA test standards are used to measure and correct for geometrical distortion and convolutional blurring, allowing high-precision, stitched measurements over large-area gratings. Development of each facet of the project is ongoing, and it remains to optimize all of the procedures and integrate them into a coordinated system.

The measurements discussed throughout the present paper, were taken with the NewView-9000 available at the ALS XROL. We have demonstrated that in the measurements with this tool, the upper limit of the groove density range achievable is $\sim 1,900$ lines/mm. This is consistent with the Abbe diffraction limit of ~ 520 nm for the microscope (the light wavelength of 570 nm) equipped with a 50 $\times$ objective (NA of 0.55).

However, we should emphasize that the described and discussed data acquisition and processing techniques are not restricted to use with this particular interferometric microscope. In fact, the techniques we are developing are generalizable to a wide range of metrology tools aside from the traditional interferometric microscopes. Application of this technique to the grating measurements using super resolution microscopy implementing advanced objectives with numerical aperture of ~ 0.9 at the wavelength of ~ 440 nm (see, for example, Refs.^{41,42} and references therein) can potentially allow to extend the achievable groove density range to $\sim 4,000$ lines/mm.

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