Ex situ metrology of x-ray diffraction gratings
(with interferometric microscopes)

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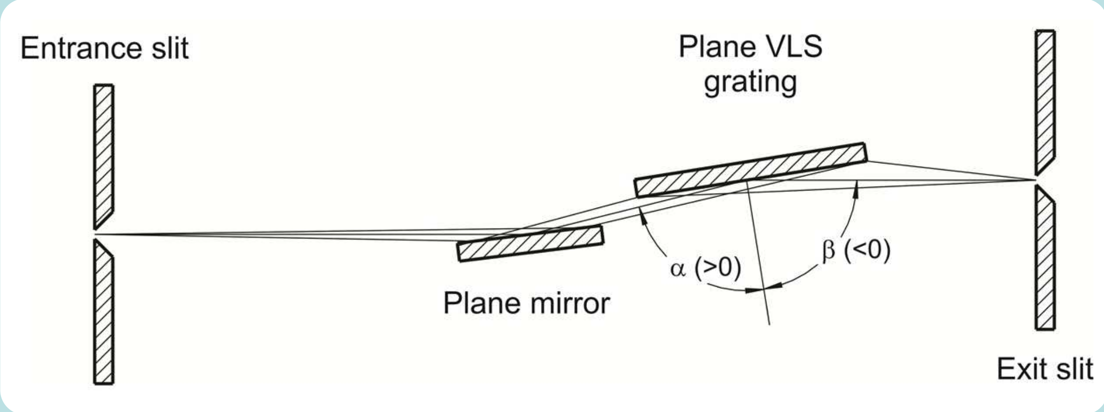
http://opticalmetrology.lbl.gov

A plane grating with a varied line spacing (VLS) in the SX700-type monochromator geometry

(The ALS MAESTRO project)



- **VLS grating does all of the focusing in the modified SX700 style monochromator.**
- **The fixed-focus parameter**

$$C = Cos\beta / Cos\alpha$$

is kept constant during the energy scan.

- **Then, the ratio of virtual-source , r', and real-source , r, distances also stays fixed.**

VLS groove density: $g = g_0 + g_1 \cdot w + g_2 \cdot w^2$

Diffraction equation: $Sin\alpha + Sin\beta = m\lambda g_0$

Focusing equation of a VLS plane grating : $\dfrac{Cos^2\alpha}{r} + \dfrac{Cos^2\beta}{r'} = m\lambda g_1$

- **Zeroing the defocusing term:**

$$Sin^2\beta\left(-\frac{1}{r}-\frac{1}{r'}\right)+Sin\beta\left(\frac{2m\lambda g_0}{r}\right)+\left[\frac{1}{r}+\frac{1}{r'}-m\lambda g_1-\frac{(2m\lambda g_1)^2}{r}\right]=0$$

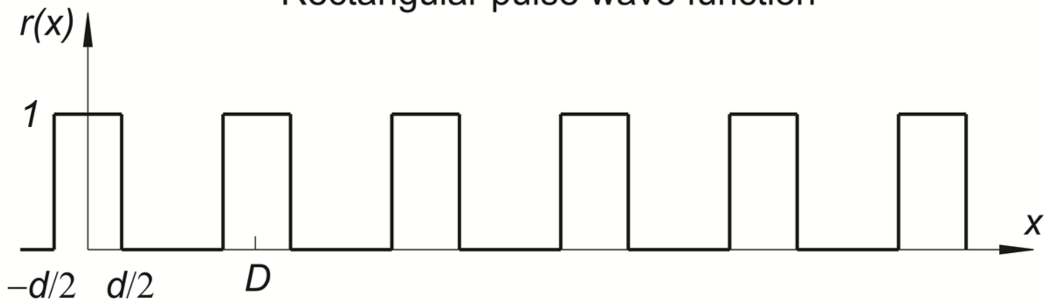
- **The second order term is chosen (usually numerically) to minimize higher order aberrations.**

? OPTICAL METROLOGY ?

Review: R. Follath and F. Senf, "*New plane-grating monochromators for third generation synchrotron radiation light sources,*" *Nucl. Instrum. and Methods*. A390, 388-394 (1997).

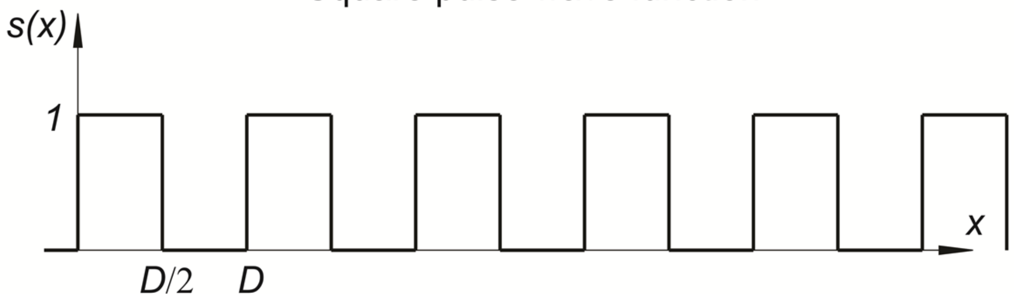
The Fourier series expansion for a rectangular pulse wave function

Rectangular pulse wave function



$$r(x)=\frac{d}{D}+\sum_{n=1}^{\infty}\frac{2}{\pi n}Sin\left(\frac{\pi n\,d}{D}\right)Cos\left(\frac{2\pi n}{D}x\right)\quad n=1\ \square\ Cos\left(\frac{2\pi}{D}x\right)$$

Square pulse wave function



$$s(x)=\frac{1}{2}+\frac{4}{\pi}\left[Sin\left(\frac{2\pi}{D}x\right)+\frac{1}{3}Sin\left(\frac{2\pi}{D}3x\right)+\frac{1}{5}Sin\left(\frac{2\pi}{D}5x\right)+\ldots\right]$$

The first (and all other!) harmonics contains information on groove density:

$$\frac{1}{D}$$

- **<u>Metrology Method:</u>**

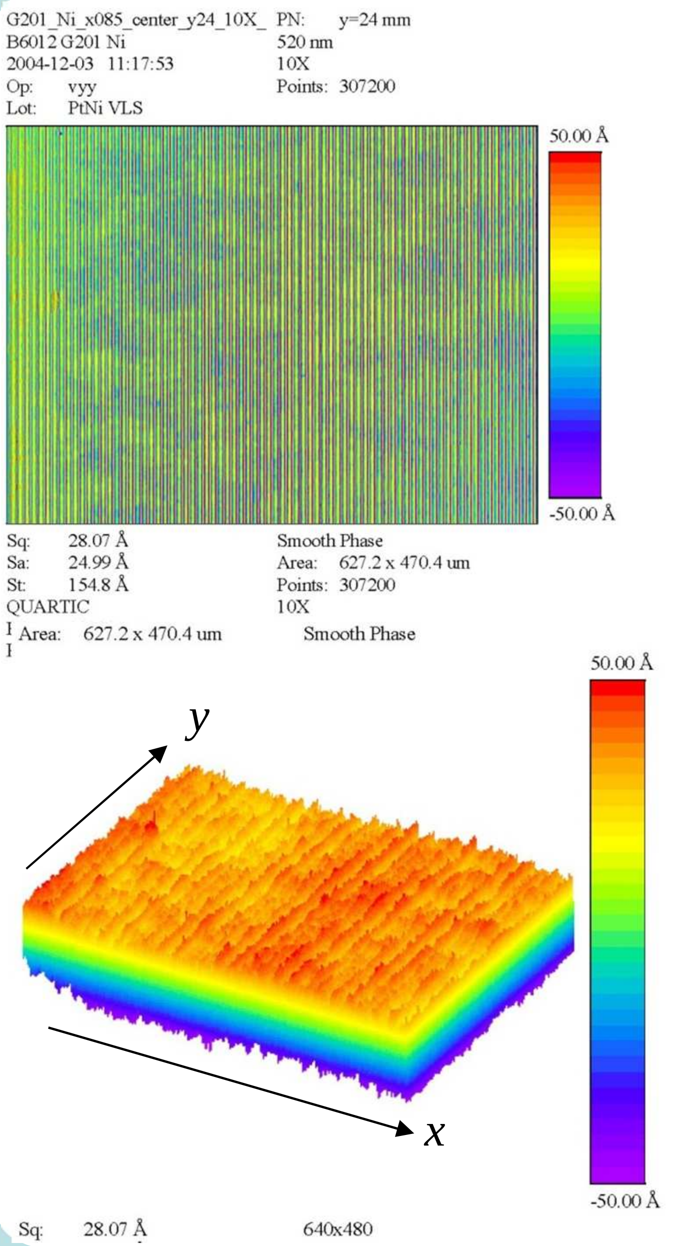
Fourier (Power Spectral Density, PSD) analysis of grating profile measurements.

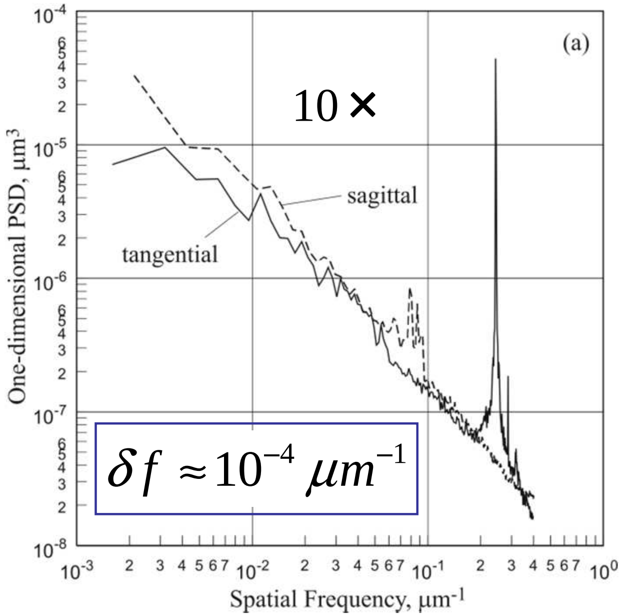
- **<u>Limiting factors:</u>**

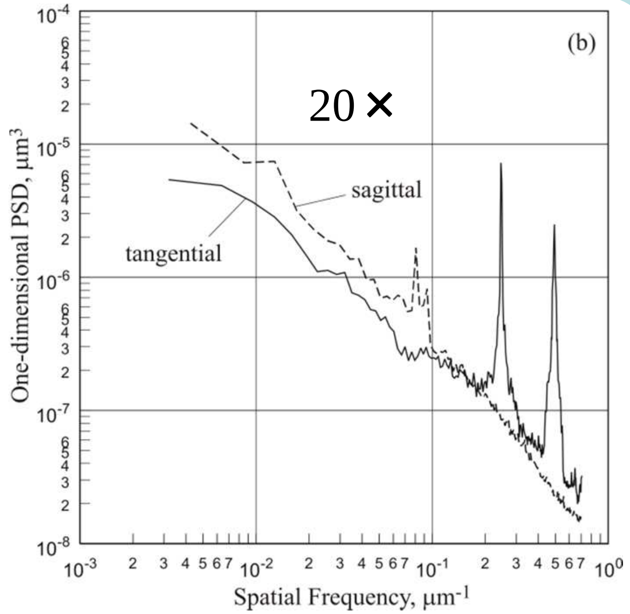
Grating profile measurements are performed over a <u>limited area</u> with a <u>limited resolution</u>

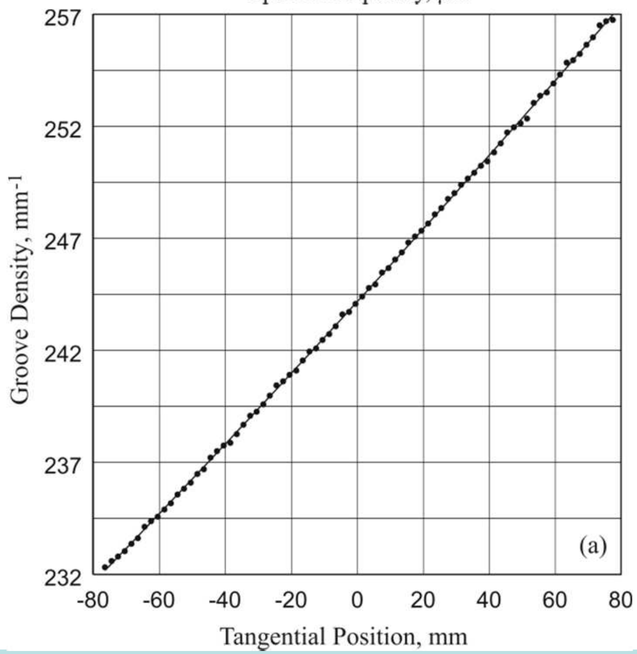
H. Stark, F. Tuteur, and J. B. Anderson, *Modern Electrical Communications. Analog, Digital, and Optical Systems*, 2nd Ed. (Prentice-Hall, London, 1988).

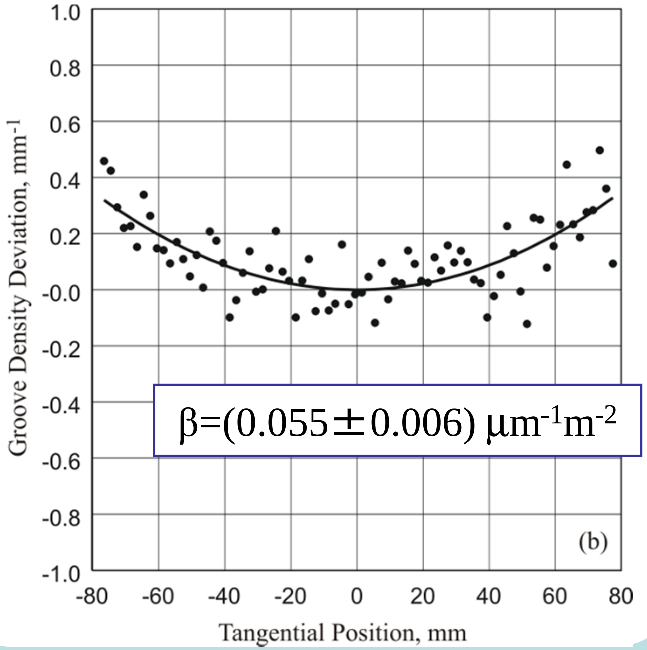
PSD measurements with MicroMap™-570 of X-ray grating with variable groove density









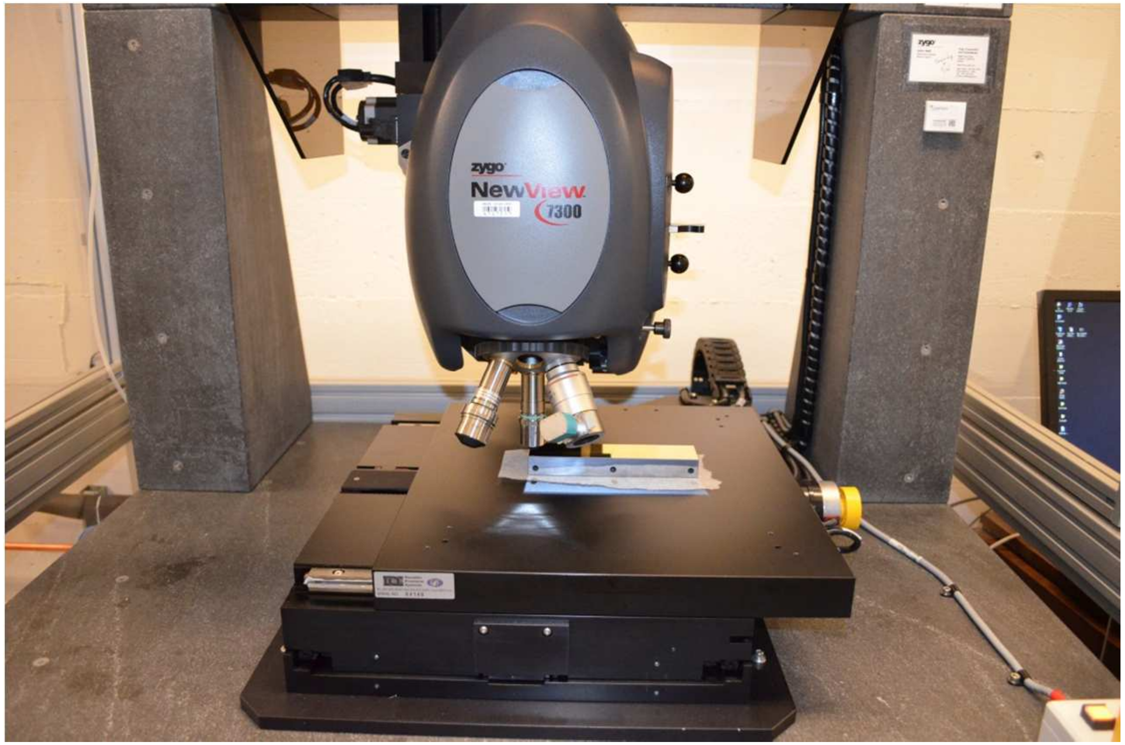


V. V. Yashchuk, A. D. Franck, S. C. Irick, M. R. Howells, A. A. MacDowell, W. R. McKinney, "*Two dimensional power spectral density measurements of X-ray optics with the Micromap interferometric microscope*," Proc. SPIE 5858, 58580A/1-12 (2005).

Characterization of VLS gratings with ZYGO NewView™-7300 interferometric microscope

ADVANCED LIGHT SOURCE

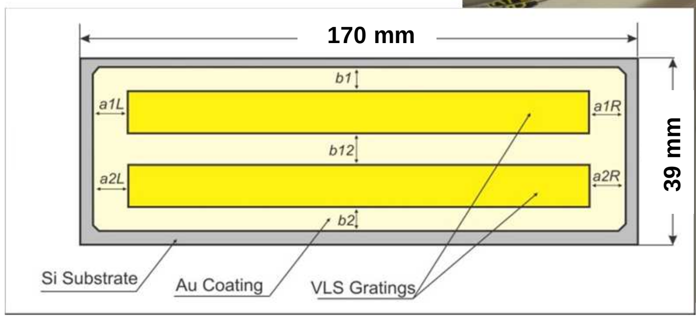
BERKELEY LAB
Lawrence Berkeley National Laboratory

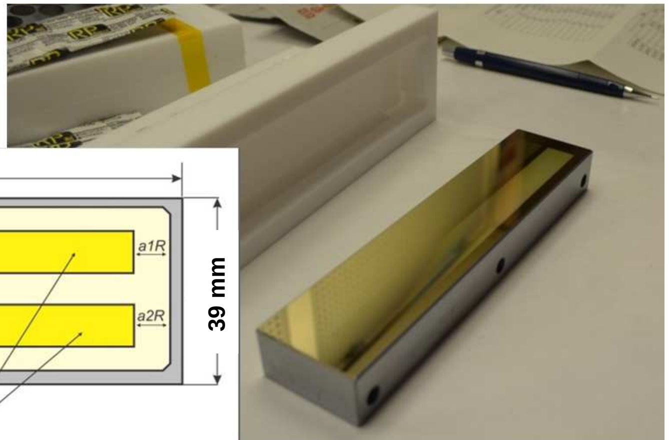


MEASURING CAPABILITIES:

- **Built-in PSD processing of the measured surface height distributions;**
- **Broad range of spatial resolution with different objectives (2.5x – 50x) and zooms (0.5x, 1x, and 2x);**
- **Multiple repeatable measurements with automated incremental translation of surface under test;**
- **Measurements with stitching…**

For MAESTRO project





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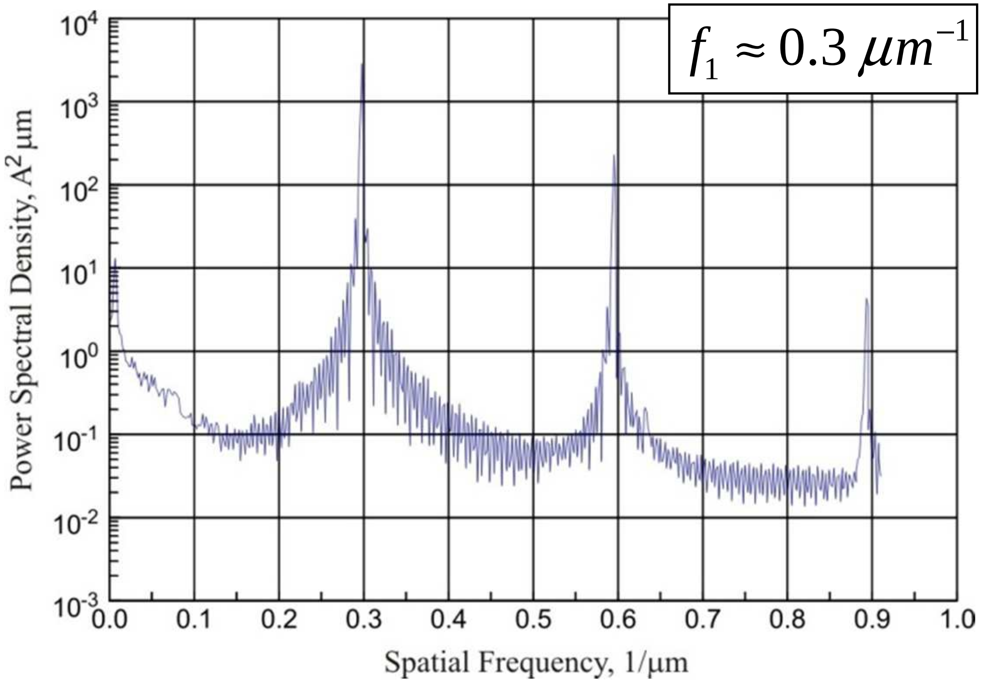
PSD spectrum of a 300-line-per-mm grating

Measured with the ZYGO NewView™-7300 interferometric microscope (λ = 0.57 nm) using 20× objective and the 1× zoom:

effective pixel size: $\Delta p \approx 0.11\,\mu m$

Nyquist frequency: $F_N \approx 0.91\,\mu m^{-1}$

number of PSD peaks: $n = 8$



PSD spectrum of the grating consists of n peaks at the spatial frequencies:

$$\omega_n = 2\pi n / D = 2\pi f_n,$$

$$1 \le n < F_N \,/\, f_1,$$

where, the Nyquist frequency of the microscope:

$$F_N = 1/2\Delta p,$$

Δp **is the effective pixel size of the CCD detector.**

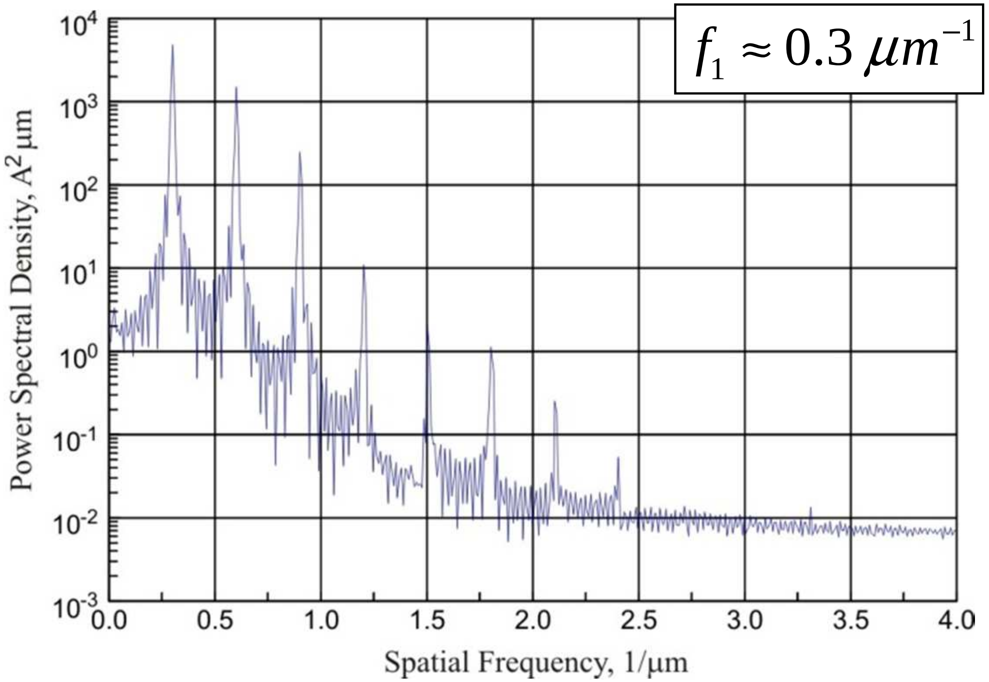
PSD spectrum of a 300-line-per-mm grating

Measured with the ZYGO NewView™-7300 interferometric microscope (λ = 0.57 nm) using 50× objective and the 2× zoom:

effective pixel size: $\Delta p \approx 0.11\,\mu m$

Nyquist frequency: $F_N \approx 0.91\,\mu m^{-1}$

number of PSD peaks: $n = 8$



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Δp **is the effective pixel size of the CCD detector.**

N.B. Microscope resolution is about

0.52 µm

determined by the diffraction limit of the objective:*

$$MTF_O(f) = \frac{2}{\pi}\left[-\Omega\sqrt{1-\Omega^2} + ArcCos\,\Omega\right]$$

where, $\Omega = \lambda f / 2NA,\ f = \sqrt{f_x^2 + f_y^2},$

NA **is the Numerical Aperture.**

* E. L. Church, P. Z. Takacs, "*Effects of optical transfer function in surface-profile measurements*," *SPIE Proc.* 1164, 46-59 (1989).

PSD spectrum of a 300-line-per-mm grating

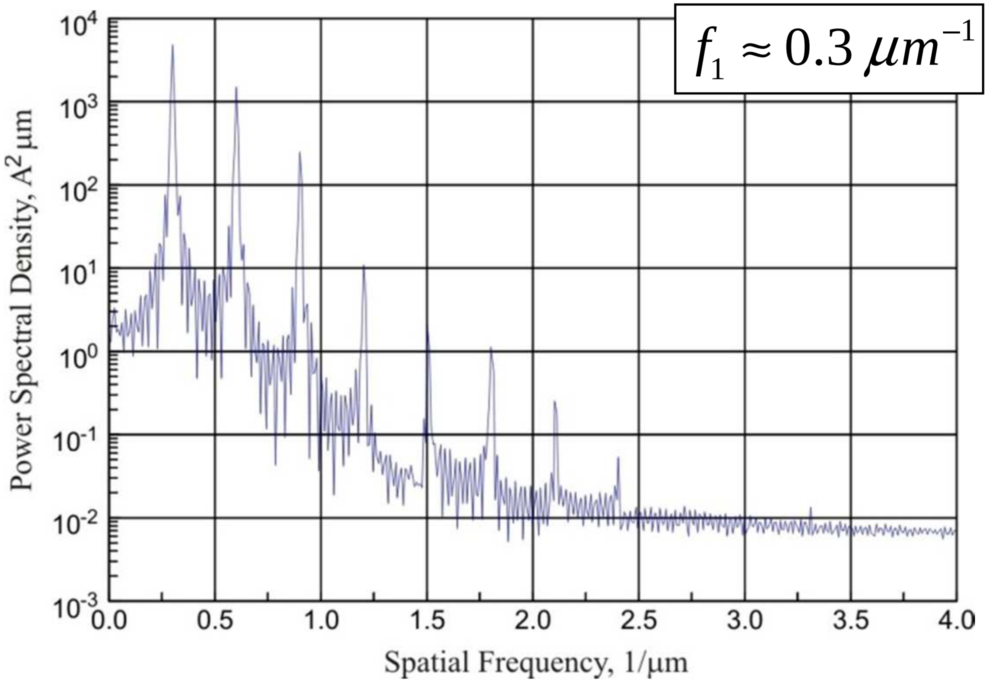
Measured with the ZYGO NewView™-7300 interferometric microscope (λ = 0.57 nm) using 50× objective and the 2× zoom:

effective pixel size: $\Delta p \approx 0.11\,\mu m$

Nyquist frequency: $F_N \approx 0.91\,\mu m^{-1}$

number of PSD peaks: $n = 8$

$f_1 \approx 0.3\,\mu m^{-1}$

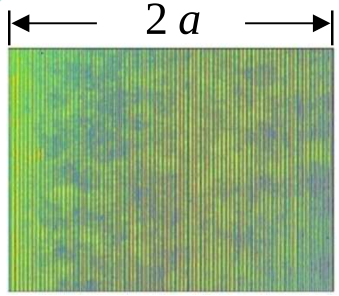


QUESTIONS:

1. **How to reliably position the PSD peaks?**
   - **Analytical fitting function…**
   - **Fitting procedure…**
2. **What is the best arrangement for the measurements?**
   - **Microscope resolution (objective, zoom)…**
   - **Measurements with stitching…**
3. **What is the reliability of the measurements?**
   - **Spatial calibration…**
   - **Cross-comparison with other methods…**

Line shape measured with a microscope with a finite size of field-of-view

If $[-a,+a]$ determines the size of the field-of-view in the direction along the grating:

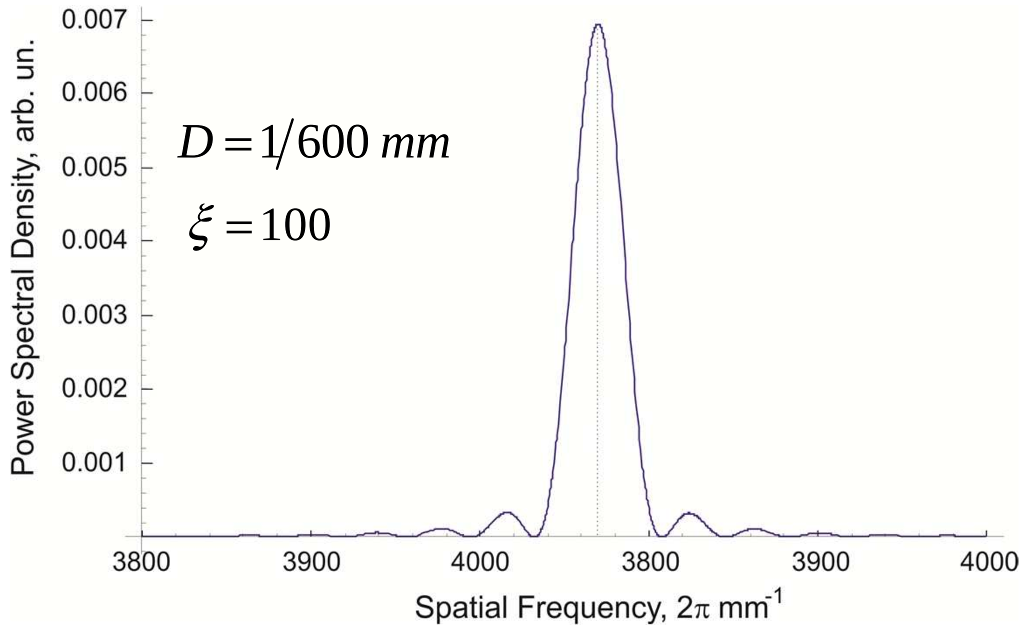


$$P_{f_1}(f) \propto I_1(f) = \left| \int_{-a}^{a} Sin\left(\frac{2\pi}{D}x\right)\exp(-i f x)dx \right|^2$$

$$= 4\left[f_1 Cos(a f_1) Sin(a f) - f Cos(a f) Sin(a f_1)\right]^2 \Big/ \left(f^2 - f_1^2\right)^2$$

$$= 4\left[\frac{2\pi}{D} Cos(\pi\xi) Sin(\frac{\xi D}{2} f) - f Cos(\frac{\xi D}{2} f) Sin(\pi\xi)\right]^2 \Bigg/ \left(f^2 - \left(\frac{2\pi}{D}\right)^2\right)^2$$

First harmonic peak in PSD spectrum



$\xi = 2a/D$ **is the number of grooves seen in the microscope's field-of-view**

If ξ is an integer number:

$$I_1(f) = 4\left[\frac{2\pi}{D} Sin\left(\frac{\xi D}{2} f\right)\right]^2 \Bigg/ \left(f^2 - \left(\frac{2\pi}{D}\right)^2\right)^2$$

$$= \left\{ 2\pi\xi \cdot Sinc\left(\frac{\xi D}{2}\left(f - \frac{2\pi}{D}\right)\right) \Big/ \left(f + \frac{2\pi}{D}\right)\right\}^2$$

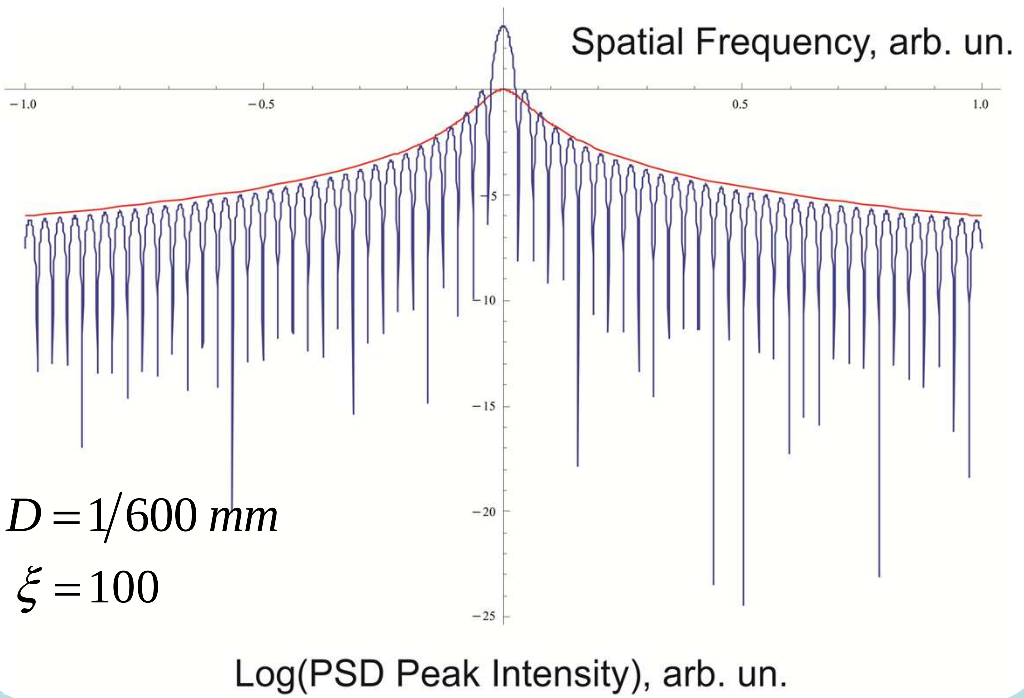
Logarithmic scale to increase the number of points included into the peak fitting

$$I_1(f) = \left\{ 2\pi\xi \cdot Sinc\left(\frac{\xi D}{2}\left(f - \frac{2\pi}{D} \right) \right) \Big/ \left(f + \frac{2\pi}{D} \right) \right\}^2$$

$$S(f) = Log\left[I_1(f) \right] = A_0 + B_0 \cdot Log\left| Sinc\left(\frac{\xi D}{2}\left(f - \frac{2\pi}{D} \right) \right) \right| + C_0 \cdot Log\left(f + \frac{2\pi}{D} \right)$$

$$= A_0 + B_0 \cdot Log\left| Sinc\left(a \cdot (f - f_1) \right) \right| + C_2 \cdot (f - f_1)$$

First harmonic peak in PSD spectrum



Problems to solve:

- **Fit in the presence of the oscillations**
- **Fit at the peak center**

Fit with the Lorentzian function:

$$L(f) \approx A_L + B_L Log\left[(w/2)^2 \Big/ f^2 + (w/2)^2 \right]$$

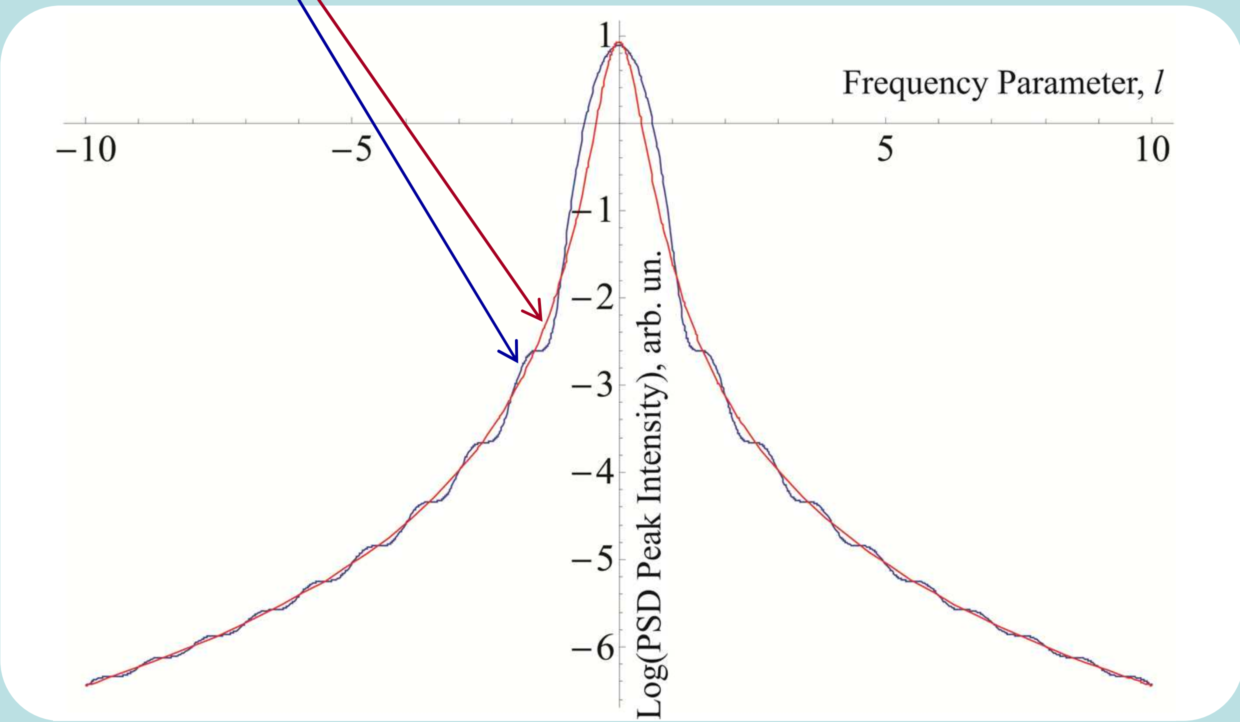
Smoothing of *Sinc*-function oscillations in discrete PSD measurements

Averaging over half of the oscillation period: $\Delta f = 2\pi/\xi D$

$$S_{Int}(f_l) = \int_{\pi l-\pi/2}^{\pi l+\pi/2} Sinc^2(x)\,\mathrm{d}x$$

$$= \frac{4Cos^2(l\pi) + (4l^2-1)\pi\left[SinIntegral(\pi - 2l\pi) + SinIntegral(\pi + 2l\pi])\right]}{(4l^2-1)\pi}$$

$$\approx A + B\cdot Log\left[\left((f-f_1)^2 + \eta\cdot(w/2)^2\right)\Big/\left((f-f_1)^2+(w/2)^2\right)^2\right] + C\cdot(f-f_1)$$



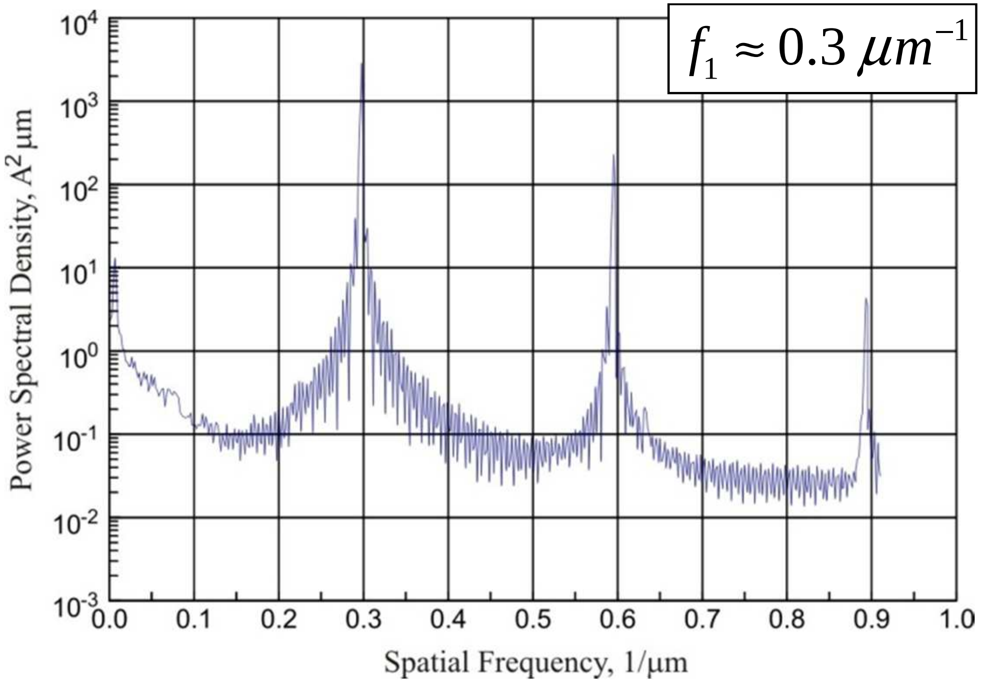
N. B. If the number of points per one grating period is just a few, the PSD measurements strongly depend on mutual alignment of the grating groove phase with respect to the pixel grid of the detector CCD camera.

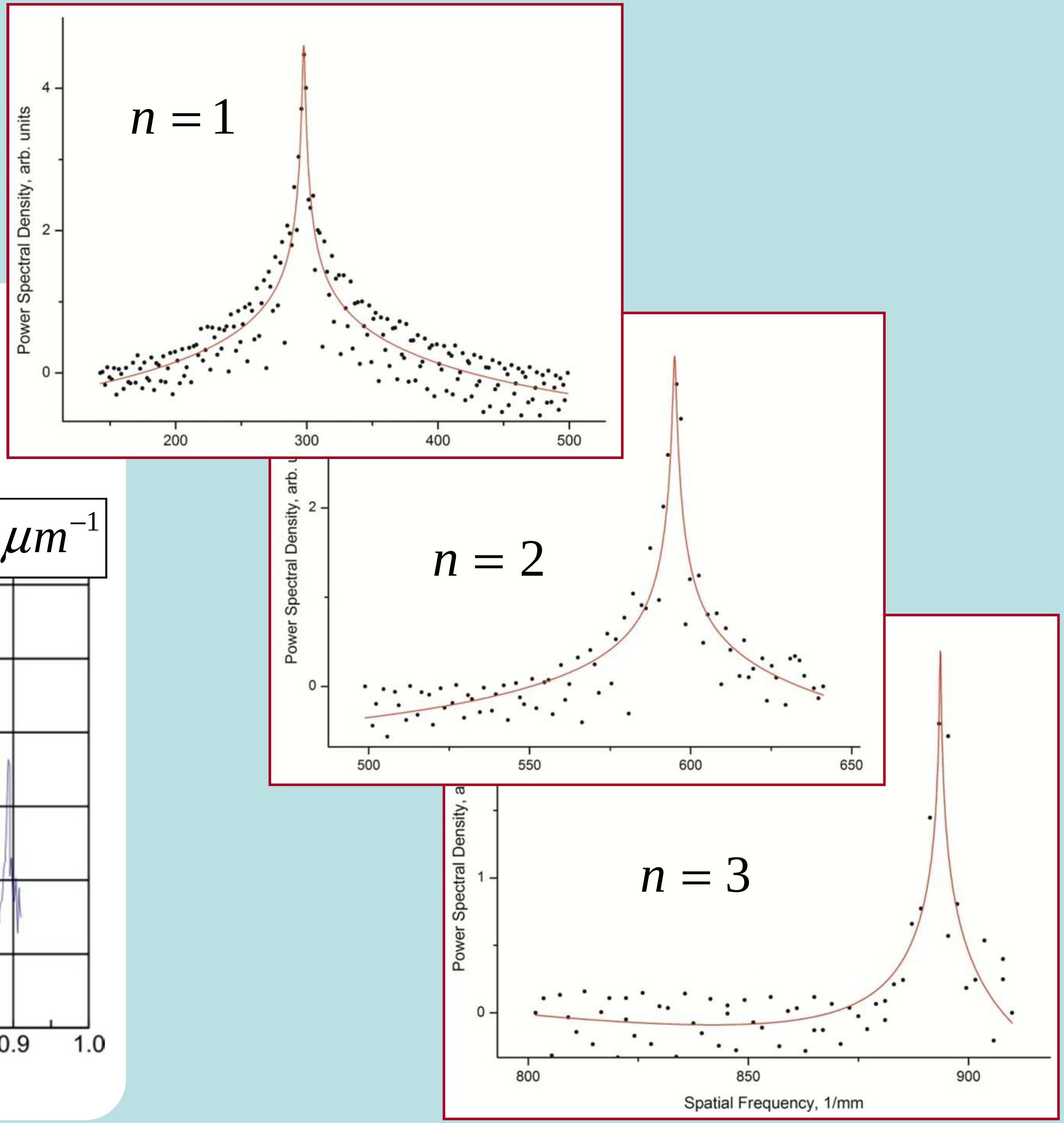
This case should be specially analyzed (in progress).

Fitting of the PSD peaks with the derived analytical function

Measured with the ZYGO NewView™-7300 interferometric microscope (λ = 0.57 nm) using 20× objective and the 1× zoom:

$f_1 \approx 0.3\ \mu m^{-1}$





$$S_{Int}(f_l) = A + B \cdot Log\left[\left((f-f_1)^2 + \eta\cdot(w/2)^2\right)\Big/\left((f-f_1)^2+(w/2)^2\right)^2\right] + C\cdot(f-f_1)$$

Evaluation of the groove density from the entire PSD spectrum

ZYGO NewView™-7300 with the 300-line-per-mm grating

20× objective and the 1× zoom

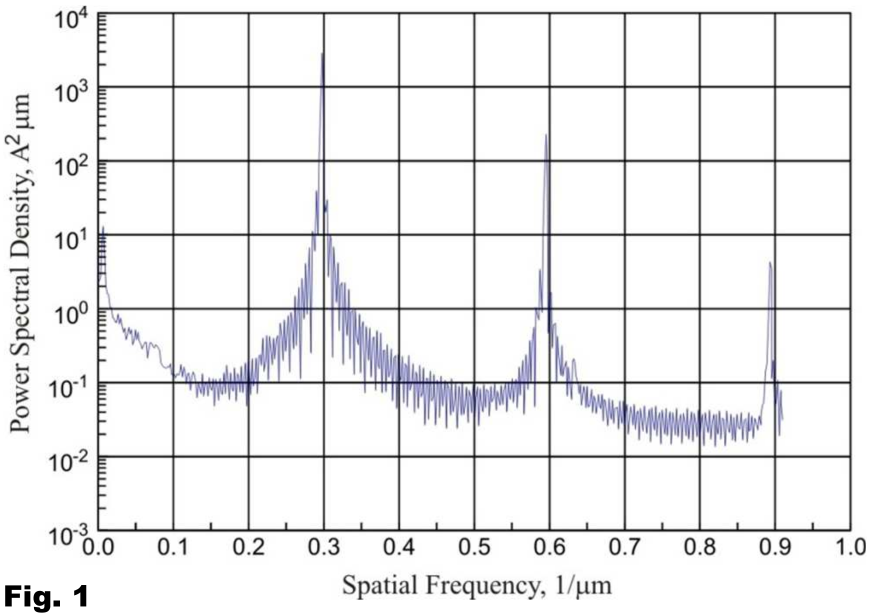


Fig. 1

50× objective and the 2× zoom

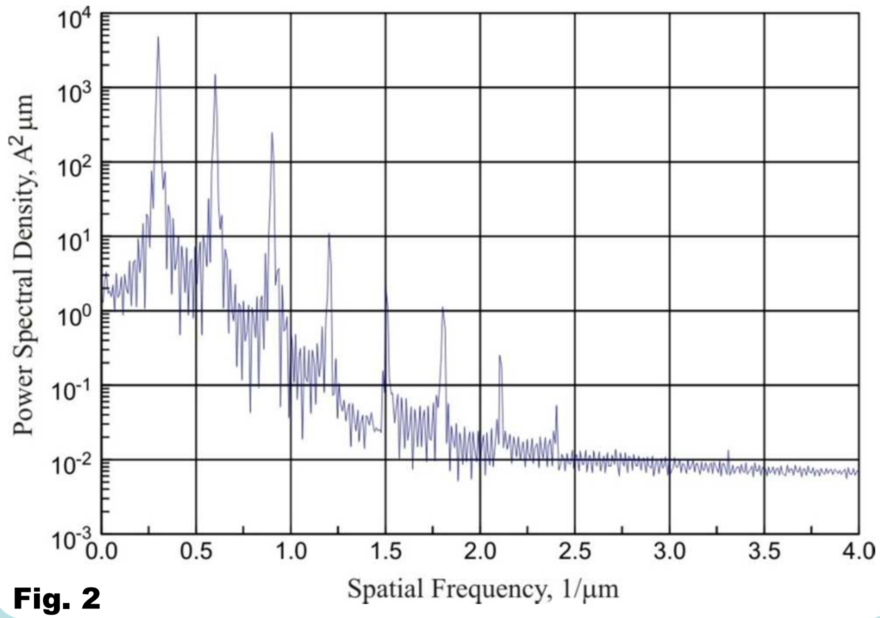


Fig. 2

n	PSD spectrum in Fig. 1		PSD spectrum in Fig. 2	
	Peak Frequency, 1/mm	Standard Error, 1/mm	Peak Frequency, 1/mm	Standard Error, 1/mm
1	297.53	0.30	302.68	1.9
2	595.01	0.40	603.80	2.3
3	893.60	0.64	905.09	1.8
4	--	--	1204.77	2.5
5	--	--	1507.83	2.2
6	--	--	1805.66	3.0
7	--	--	2104.72	4.5
8	--	--	2395.83	12.5

$$S_{Int}(f_l) = A + B \cdot Log\left[\left((f-f_1)^2 + \eta \cdot (w/2)^2\right) \Big/ \left((f-f_1)^2 + (w/2)^2\right)^2\right] + C \cdot (f - f_1)$$

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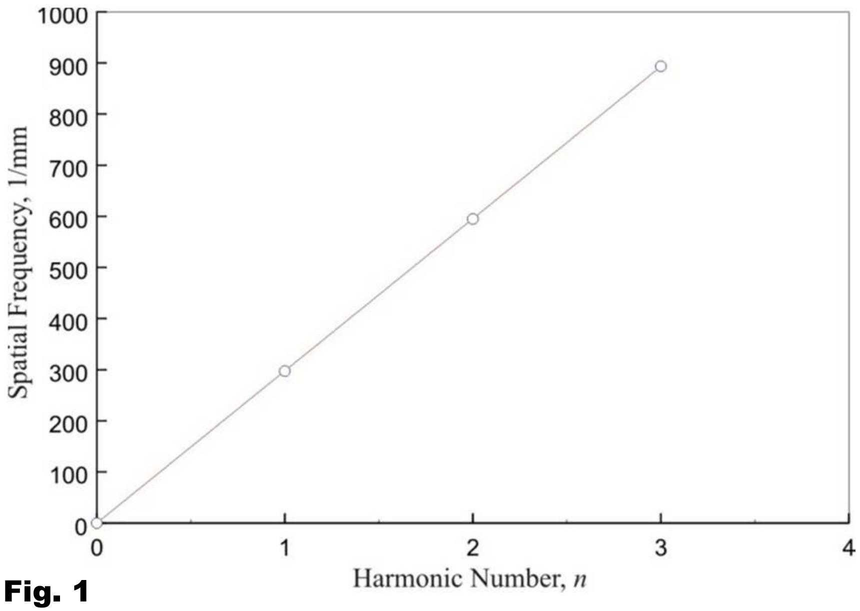

Fig. 1

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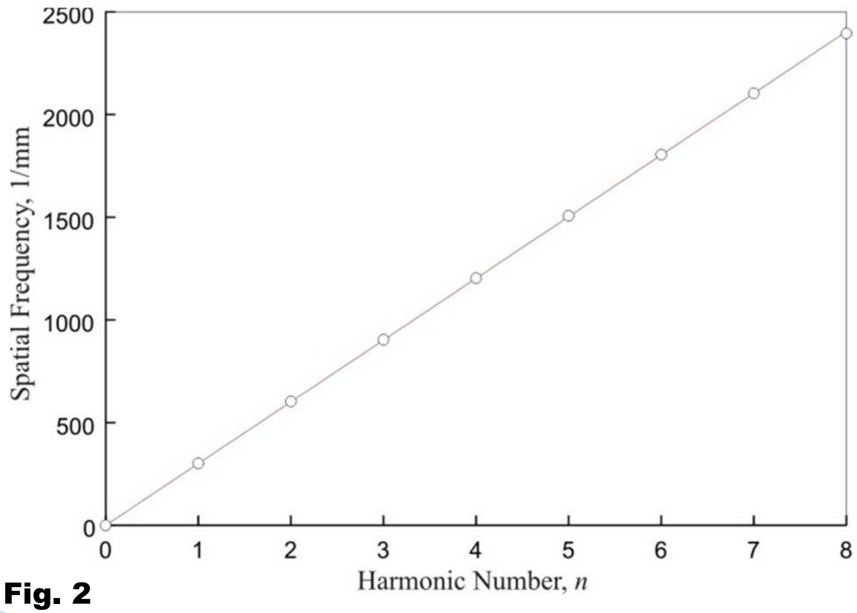

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Averaged Density	297.74 lines/mm	0.10 lines/mm	301.27 lines/mm	0.19 lines/mm

V. V. Yashchuk, "*Positioning errors of pencil-beam interferometers for long-trace profilers*," Proc. SPIE 6317, 6317-10/1-12 (2006).

Number of grooves vs Number of peaks

ZYGO NewView™-7300 with the 300-line-per-mm grating

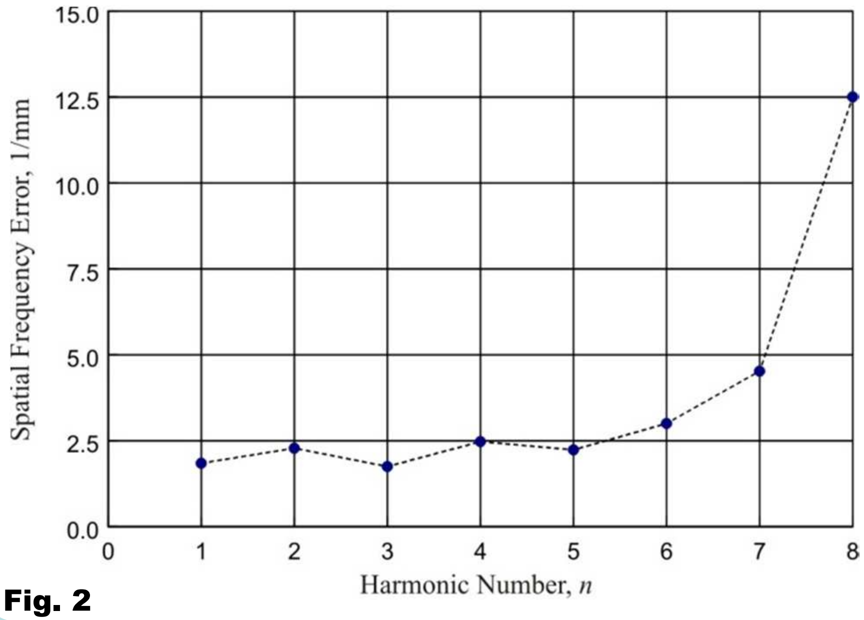
OBSERVATION:

The linear fit of data in Fig. 2 provides an improvement of the standard error by a factor of ~10.

- **Fitting with weighting accounts for the standard errors of the peak frequency values;**
- **Statistical significance of a peak in the final value of the groove density is proportional to the harmonic number, *n*.**

The standard error of a peak frequency is inversely proportional to the linear size of the field of view.*

50× objective and the 2× zoom



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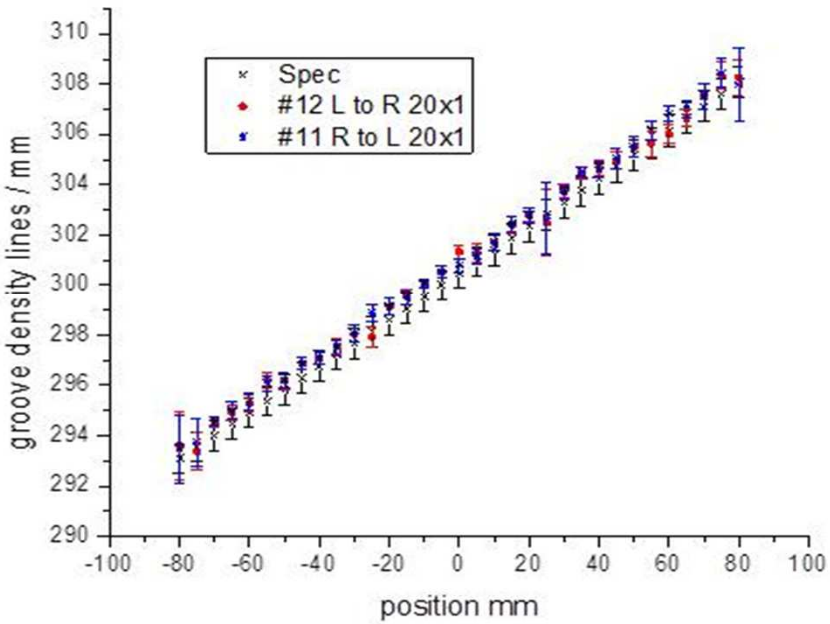
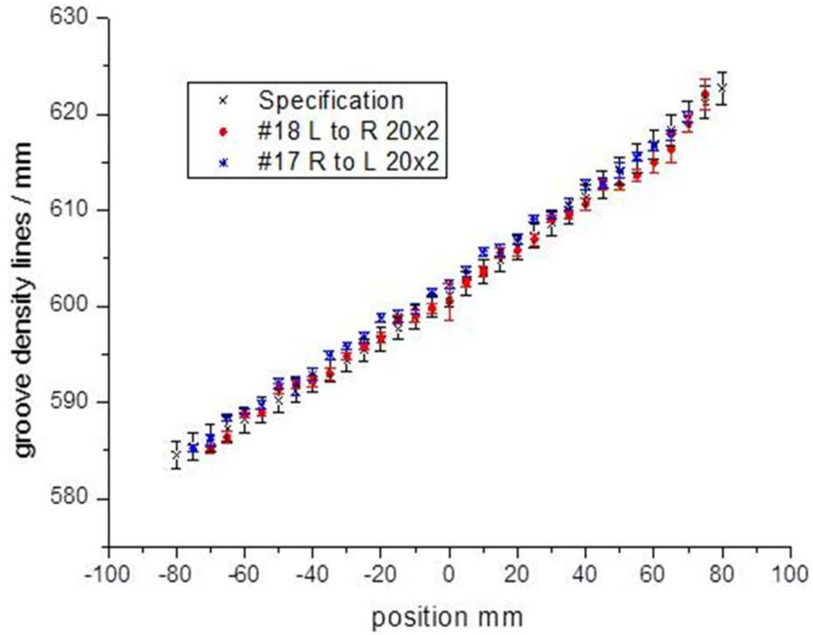
* D. L. Voronov, R. Cambie, R. M. Feshchenko, E. Gullikson, H. A. Padmore, A. V. Vinogradov, V. V. Yashchuk, *Development of an ultra-high resolution diffraction grating for soft X-rays,* Proc. of SPIE Vol. 6705, 67050E (2007).

Cross-comparison with vendor metrology

300-lines-per-mm grating



600-lines-per-mm grating



	Specification (mm)	Measurement (mm)	Specification (mm)	Measurement (mm)
g_0	300 ± 0.6 mm^{-1}	300.87 ± 0.05 mm^{-1}	600 ± 1.2 mm^{-1}	602.02 ± 0.11 mm^{-1}
g_1	0.0935 ± 0.00047 mm^{-2}	0.0920 ± 0.0008 mm^{-2}	0.235 ± 0.001 mm^{-2}	0.23091 ± 0.0018 mm^{-2}
g_2	$1.9\times10^{-5} \pm 0.29\times10^{-5}$ mm^{-3}	$2.08\times10^{-5} \pm 1.4\times10^{-5}$ mm^{-3}	$3.8\times10^{-5} \pm 0.57\times10^{-5}$ mm^{-3}	$9.07\times10^{-5} \pm 3.1\times10^{-5}$ mm^{-3}

"truth" is hard to know; it may also have uncertainty...

Conclusions

Results obtained:

- An analytical expression for the shape of the first harmonic peak in the PSD spectrum of a diffraction grating has been derived.
- Based on the analytical expression, an approximate fitting function has been suggested.
- The developed fitting procedure has been successfully applied to the PSD metrology of a 300-lines-per-mm grating.
- Cross-comparison with the vendor metrology has suggested for high reliability of the lateral calibration of the interferometric microscope used for the measurements.
- A possibility to get valuable data on the groove density for a grating with a pitch smaller than the microscope resolution has been demonstrated.

Questions to be investigated (research in progress):

- Dependence of the PSD measurements on mutual alignment of the grating groove phase with respect to the pixel grid of the detector CCD camera in the case when the number of points per one grating period is just a few.
- Theory of groove density measurements for a grating with a pitch smaller than the microscope's resolution (e.g., via use of the aliasing effect).
- Ways to increase accuracy: Measurements with stitching… to test stitching!!!

  (Note that the first try has failed…)

"Enjoy your achievements as well as your plans"

Max Ehrmann, "Desiderate" (1948)

Acknowledgements

We are grateful to Tony Warwick for providing the MAESTRO grating for optical metrology.

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"Measurement science is not, however, purely the preserve of scientists. It is something of vital importance to us all. The intricate but invisible network of services, suppliers, and communications upon which **we are all dependent relies on metrology for its efficient and reliable operation.**"

Bureau International des Poids et Mesures (BIPM)
[Eng.: International Bureau of Weights and Measures]
http://www.bipm.org/en/convention/wmd/2004/