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**Automated suppression of errors in LTP-II slope measurements
with x-ray optics.**

Part1: Review of LTP errors and methods for the error reduction

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ABSTRACT

Systematic error and instrumental drift are the major limiting factors of sub-microradian slope metrology with state-of-the-art x-ray optics. Significant suppression of the errors can be achieved by using an optimal measurement strategy suggested in [Rev. Sci. Instrum. 80, 115101 (2009)]. With this series of LSBL Notes, we report on development of an automated, kinematic, rotational system that provides fully controlled flipping, tilting, and shifting of a surface under test. The system is integrated into the Advanced Light Source long trace profiler, LTP-II, allowing for complete realization of the advantages of the optimal measurement strategy method. We provide details of the system's design, operational control and data acquisition. The high performance of the system is demonstrated via the results of high precision measurements with a spherical test mirror.

Keywords: surface slope metrology, drift error, systematic error, optimal scanning, metrology of x-ray optics, deflectometry

1. INTRODUCTION

Development, characterization, and application of state-of-the-art X-ray optics for 3rd and 4th generation X-ray light sources with a level of surface slope precision of 0.1-0.2 μrad requires the development of adequate dedicated metrology instrumentation and methods [1-3]. The best performing slope measuring profilers at synchrotron facilities, such as the Nanometer Optical Component Measuring Machines (NOM) at Helmholtz Zentrum Berlin (HZB)/BESSY-II (Germany) [4-7] and at the Diamond Light Source (UK) [8], as well as Long Trace Profilers (LTP) at SPring-8 (Japan) [9], at ESRF [10,11], at SOLEIL [12,13] (France), and at the ALS (U.S.A.) [14-16] come close to the required precision. The high performance of the instruments is based on thorough suppression of the measurement errors due to random noise, systematic effects, and instrumental drifts. A comprehensive analysis of errors of slope measurements and discussion of methods for decreasing the errors can be found, e.g., in Refs. [16-21].

Significant suppression of the errors (in particular, errors associated with instrumental and set-up drifts) can be achieved by using an optimal measurement strategy suggested and comprehensively analyzed in Ref. [20]. With the present Note, we start reporting on development of an automated, kinematic, rotational system that provides fully controlled flipping, tilting, and shifting of a surface under test. The system is integrated into the Advanced Light Source long trace profiler, LTP-II, allowing for complete realization of the advantages of the optimal measurement strategy method.

We start here with analysis of the major contributors to the LTP error budget and a brief discussion of the methods developed to decrease the errors. The optimal measurement (scanning)

strategy method, which we have successfully used to significantly suppress LTP drift error, is briefly overviewed in Sec. 3.

In the next Notes we will summarize the requirements and crucial specifications for a system that would realize the advantages of the optimal scanning method, and allow also for effective suppression of random and systematic errors. We will also provide details of the system's design, operational control and data acquisition. The high performance of the system will be demonstrated the results of high precision measurements with a spherical test mirror. Finally, we will point to the problems of surface slope profilometers that still wait for solutions, and project directions for further investigation.

2. ANALYSIS OF LTP ERRORS

In this section, we briefly overview the major error sources and methods developed to minimize the contributions of the errors to the surface slope measurements with emphasis on our experience measuring high quality x-ray optics with the ALS LTP-II [14-16].

The main difference between an LTP II and an instrument of the first generation is the addition of a reference arm that records a reference slope signal from a stationary reference mirror [22-24]. A similar approach has been used in a dual-beam laser deflection sensor described in Ref. [25]. In the LTP-II, the reference trace is subtracted from the sample trace, providing data basically free of errors (such as the ones due to wobbling of the LTP carriage and pointing instability of the laser beam) that are common to the sample and the reference channels. As a result, LTPs with the optical reference channel became capable of slope measurements with accuracy of about 1 μrad . Paradoxically, further improvement of LTP performance to the level of modern requirements of $\sim 0.1 \mu\text{rad}$ must overcome a number of disadvantages inherent to the optical reference channel (see, e.g., [14]).

A slope measurement of a surface under test (SUT) provides the dependence of the surface slope $\alpha(x)$ on a position x . The measurement is performed with an LTP by scanning the position variable over the discrete points x_i , $i = 0, 1, \dots, (I-1)$, uniformly distributed over the range of interest, e.g., the SUT clear aperture. Generally a result of slope measurement can be expressed as

$$\alpha_M(x_i) = \alpha(x_i) + R(x_i) + S(\alpha(x_i), x_i) + D(x_i(t)), \quad (1)$$

where the measured slope $\alpha_M(x_i)$ is affected by random error $R(x_i)$, systematic error $S(\alpha(x_i), x_i)$, and drift $D(x_i(t))$ of the measurement instrument and experimental setup. Below we analyze errors specific for slope measurements with the ALS LTP-II.

2.1. Random Errors

Random errors, depicted in Eq. (1) as $R(x_i)$, are caused by unpredictable fluctuations in the readings due to the limited precision of the instrument or may be due to the random character of spurious effects. Note that in spite of the fact that there is no correlation between the random error and the measured position, we still show in Eq. (1) a more general dependence of random error on x_i that allows, e.g., a possible positional dependence of the variance of the random error.

The main source of random error of an LTP-II is air convection in the reference and sample channels caused by temperature gradients and air flow [26]. Due to air convection (turbulence) the refractive index of the air along the optical paths changes, leading to pointing instability of the light beams. Because the optical paths of the sample and the reference beams are different, the corresponding errors do not correlate, and cannot be accounted by the optical reference channel.

The intensity of the air convection, as well as the overall stability of an optical profiler system, are strongly correlated with environmental conditions in the lab. Currently, the ALS OML air-conditioner keeps the room temperature stable at approximately 20°C with about a ± 120 mK periodic (~ 12 min period) variation determined by the switch-on/-off cycle of the OML air-conditioner. Additional temperature insulation of the LTP with a surrounding hutch keeps temperature variation over the measuring set-up of ~ 20 mK [27]. The resulting random error of the slope reading in the ALS LTP-II reference channel is still rather large of about $0.3 \mu\text{rad}/\text{Hz}^{1/2}$ (after averaging over 10 sequential measurements taken over an interval of about 1 second).

The air-convection error can be significantly suppressed by additional shielding of the LTP optical paths [26]. However, it is difficult, if not impossible, to apply adequate shielding to the reference channel that is subject to continuous change during a scan.

Due to the intrinsic low frequency character of the air convection noise (with characteristic frequencies of 0.1-1 Hz [26]), simple suppression of the noise by averaging the repeated measurements is inefficient. The frequency spectrum of the noise (and, therefore, the efficiency of averaging) can be significantly increased by using an air blowing technique described in Ref. [26].

Note that possible radical (but very expensive and impractical) solutions to the problems related to variation of optical paths due to the environmental factors (temperature gradients, air density and humidity changes) would be an LTP designed for operation under vacuum [17] or in a noble-gas atmosphere.

Below, we show that suppression of the errors due to systematic effects and instrumental drift can be achieved by averaging of multiple measurements performed under controlled changes of the parameters of the experimental set-up and scanning. In this case, the low frequency random noise is also effectively averaged out because of the significantly long time intervals between the sequential scans.

2.2. Systematic Errors

Performance of the ALS LTP-II is still limited by systematic errors [14,15], which are systematically reproduced in identical scans and, therefore, cannot be suppressed by averaging over repeated measurements performed with an unchanged experimental arrangement. In general, the systematic error is specific for a particular measurement arrangement as it is accounted in the definition (1) with the term $S(\alpha(x_i), x_i)$ that depends not only on position but also on the measured value itself. Note that the only systematic error of the LTP-II that is accounted by the optical reference channel is due to profile imperfections of the ceramic beam, causing a systematic wobbling of the LTP carriage up to $10 \mu\text{rad}$.

In order to totally account for other major sources of LTP systematic errors, non-ideality of the photo-detector [19], ‘ghost’ effects due to cross contamination of sample and reference signal into one another [28], imperfections of the LTP optical elements [14-19], and non-linearity of the

LTP position-to-slope conversion, a sophisticated calibration of the instrument for a specific experimental arrangement is required [13,21,27,29]. Nevertheless, a partial suppression of most of the systematic error is still possible without a precision calibration.

In our old LTP with a one-dimensional (1D) photo-diode array (PDA) as a detector, the PDA pixel-to-pixel ($25\ \mu\text{m} \times 2.5\ \text{mm}$) photo-response non-uniformity, which was about $\sim 2\%$, led to an LTP systematic error of $\sim 0.3\ \mu\text{rad}$ (rms) [14,19]. An equal systematic error was also due to PDA pixel pitch non-uniformity ($\sim 10\%$). Both these errors are effectively suppressed to a level of below $0.1\ \mu\text{rad}$ with a 2D-CCD-based detector [9,14,19,30] with a significantly small pixel size ($7.4 \times 7.4\ \mu\text{m}^2$ in the upgraded ALS LTP-II [14]), and a flat-field calibration of the photo-response non-uniformity [29].

The ‘ghost’ effect arises when there is unavoidable cross-contamination of the LTP sample and reference signals into one another. Such a situation often happens in the measurements of a significantly curved optic with an LTP with a 1D PDA detector. The ‘ghost’ effect leads to a systematic perturbation in the recorded interference patterns and, therefore, a systematic variation of the measured slope trace. Perturbations of about $1\text{--}2\ \mu\text{rad}$ and even larger have been observed with a cylindrically shaped X-ray mirror and with a mirror having a toroidal surface figure [28]. A relatively simple method for effective suppression of the ‘ghost’ effect has been suggested in Ref. [28]. The method employs separate measurement of the ‘ghost’-effect-related interference patterns in the sample and the reference arms and then subtraction of the ‘ghost’ patterns from the sample and the reference interference patterns. Note that the procedure preserves the advantage of simultaneously measuring the sample and reference signals.

Imperfections of optical homogeneity of materials and surface quality of the LTP optical elements (beam splitters, Dove prism, quarter wave plate, Fourier lens, folding mirrors) have been shown to produce a systematic error of $0.2\text{--}0.9\ \mu\text{rad}$, depending on the curvature of the SUT [14]. In a slope trace measured with the LTP, these systematic errors appear as local (relatively high spatial frequency) perturbations.

Besides the significant improvement of quality of the optical elements (that can be rather expensive), there is an experimental way to decrease the systematic error due to imperfections of the LTP optics. For this one should average multiple measurements with different alignments (tilt in the tangential and the sagittal directions), longitudinal positions, and orientations of the SUT with respect to the LTP. Because of differences in the optical paths of the LTP beams through the LTP sensor optics, the systematic perturbations in these measurements will appear at different places of the slope trace and, therefore, will be effectively averaged out. Practically, in this way, the high spatial frequency systematic error of the LTP-II can be suppressed to the level of 0.1 to $0.4\ \mu\text{rad}$, depending on the curvature of the SUT [14,16].

2.3. Drift Errors

The drift error appears as a very slow temporal variation of the measured quantity with a characteristic time comparable to the duration of the measurements. It is, in some sense, in between random noise and systematic error. Drift error is difficult to suppress by averaging over multiple identical scans carried out over a reasonable time. In contrast to systematic errors, drifts are not stable enough to be accounted for by a precise calibration or by a simple change of the experimental arrangement.

Drift error is distinguished by its very low frequencies, requiring very long averaging times. These long times make suppression by multiple scans difficult for this error. However, it appears still to be possible.

Without loss of generality, a slow drift described with the term $D(x_i(t))$ in Eq. (1) can be expanded as a MacLaurin series in t ,

$$D(x_i(t)) = D(t) = \sum_{p=0}^{\infty} \frac{D^{(n)}(0)}{p!} t^p. \quad (2)$$

During an LTP scan, only a few first terms in the sum (2) are practically important. In the next section, we will briefly overview an experimental method, described in detail in Ref. [20], for the effective suppression of spurious effects caused by a drift presented by a certain power polynomial in Eq. (2).

The main sources of drift error in LTP measurements are the variations of the environmental conditions (temperature and, in some degree, humidity in the lab), and the inherent temporal instabilities of the experimental setup (e.g., mechanical instability of the mirror mounting and alignment) [1,5,20]. In order to decrease the effect of ambient temperature variation on the measurements, the ALS LTP-II set-up is placed in a one layer hutch. Unfortunately, inside the hutch [14,17], there are a number of heat sources, such as the diode-laser unit, carriage driving motor, CCD camera, and the heat sinks and fans of the temperature stabilized systems of the CCD camera and tiltmeters. These sources, as well as air flow of the air bearing system and stepper motors can potentially lead to temporal instabilities of various LTP components and therefore to drift errors. Note that with a hutch, one also increases the effective time constant of the temperature stabilization of the set-up inside the hutch that can increase the delay time for system stabilization before starting the measurements.

In an LTP-II with a classical optical schematic of a pencil-beam interferometer, two 90°-roof-prisms are used to produce two parallel beams with desired phase shift of π . Unfortunately, temperature instability of the prism mounts can cause the optical path difference between the two beams to change by several nanometers [14,16,20]. The resultant shift in the fringe position for this error is on the order of several microradians. Different π -phase shifters that are basically insensitive to the temperature variation have been discussed in Refs. [31,32]. The most simple one is based on a step-plate [15,31,32]. Note that an LTP schematic with a single Gaussian beam is also possible [15].

A change of temperature of the LTP diode laser leads to variations of wavelength and direction (pointing) of the emitted light beam [33]. For the usual experimental arrangement of the ALS LTP-II, the resulting drift of the laser beam direction can be as large as 5 $\mu\text{rad}/\text{hour}$ [14]. Because of the difference of the optical paths of reference and sample beams and non-ideality of the LTP optics, the reference channel accounts for the laser pointing instability only to a certain extent, leaving a noticeable contribution to the drift error. Further improvement can be obtained by replacing the laser with a laser system less sensitive to the surrounding environmental conditions. Pointing instability of different lasers, a diode laser similar to one used with the existing ALS LTP-II, an intensity stabilized HeNe laser and a fiber coupled temperature stabilized diode laser, have been experimentally investigated in Refs [26,33]. For the LTP laser, the low frequency (≤ 1 Hz) variations of laser pointing are characterized with a pointing instability of ~ 0.3 μrad (rms). A fiber coupled laser has demonstrated the best stability of ~ 0.1

μrad (rms) that corresponds to the laser specification of $\sim 0.1 \mu\text{rad/K}$ [34]. The advantages of a fiber coupled diode laser have been realized, e.g., in the SPring-8 LTP [9].

Temperature fluctuations of the LTP laser wavelength can also contribute to the LTP error budget via a dependence of the effective pixel optical center on the wavelength of light. Such dependence with a magnitude of $\sim 0.01 \mu\text{m/nm}$ has been experimentally observed with a CCD camera with a pixel pitch of $24 \mu\text{m}$ [35]. A reasonable temperature stabilization of the LTP laser system would make the effect negligible.

3. OPTIMAL SCANNING STRATEGY METHOD

The experimental method for effective suppression of the spurious effects in slope measurements caused by slow instrumental drifts was suggested and first demonstrated in Ref. [20]. The method is based on optimal scanning strategies for multiple measurements analytically derived in Ref. [20]. A slope trace measurement run performed according to an optimal scanning strategy consists of a number, S , of repeatable scans arranged with sequential reversal of the direction of scanning towards increase or decrease in x_i and/or the orientation of the SUT in respect to the LTP. Such a run provides repeatable measurements at a certain point x_i at a sequence of time moments $t_i(s)$, where s is the scan number ($s=1, 2, \dots, S$), specially arranged to anti-correlate with the temporal dependence of the drift.

Denoting the directionality of the s^{th} scan with r_s ,

$$r_s = \begin{cases} +1 & \text{if the } s\text{-th scan is performed in the forward direction,} \\ -1 & \text{if the } s\text{-th scan is performed in the backward direction,} \end{cases} \quad (3)$$

an optimal scanning strategy suitable to suppress the polynomial drift error up to the power p [see Eq. (2)] should satisfy equality [20]:

$$\sum_{s=1}^{S=2^p} r_s s^{p-1} = 0. \quad (4)$$

It can be shown that for any natural number p , Eq. (4) has a solution [20]. Practically interesting solutions for the few lower order polynomials are depicted below.

Optimal scanning strategies, suitable for suppression of a linear drift, are obvious:

$$r_s(1) = \pm\{1, -1\}. \quad (5)$$

Then, the suppression of drifts of the second order would require

$$r_s(2) = \pm\{1, -1, -1, 1\}, \quad (6)$$

for third order,

$$r_s(3) = \pm\{1, -1, -1, 1, -1, 1, 1, -1\}, \quad (7)$$

Solutions (5-7) suggest that the suppression of any order drift automatically suppresses the lower orders.

There is no apparent preferred directionality of the scans, so it is natural that if the set $\{r_s\}$ is a solution then the set $-\{r_s\}$ is also a solution. Denoting the positive solution for the p^{th} order drift

suppression as $\{r_s^+(p)\}$ and the negative solution as $\{r_s^-(p)\}$, the general recursion relation [20] between the sets $\{r_s^\pm(p+1)\}$ and $\{r_s^\pm(p)\}$ is

$$\{r_s^\pm(p+1)\} = \pm \{r_s^+(p), r_s^-(p)\}. \quad (8)$$

For the case when only the scanning direction is reversed, the corresponding suppression factor can be estimated [20] as a ratio of peak-to-valley variations of the major terms of the drift error of the optimized and non-optimized runs of the same total number of scans:

$$\xi \approx 8 \cdot 2^p / p. \quad (9)$$

The estimation (9) shows that suppression factor, ξ , rapidly increases with increase of p for $p \geq 2$.

Absolute zeroing of the drift-related errors is achieved with a strategy that includes simultaneous reversals of the direction of the LTP scanning and the orientation of the SUT with respect to the LTP [20]. Therefore, the most efficient suppression of drift error (in fact, identical zeroing of polynomial drifts up to a desired order) is obtained with sequential scans with optimal reversing of the sign of the measuring quantity (surface slope) without changing the sign of the drift error contribution. The optimal sequences of the sign reversals obey the same identity as the one derived for reversing the direction of scanning, Eq. (4).

Note that the derived optimal sequences of the reversals also describe the optimal square waveforms for a drift-free multichannel phase-sensitive detection discussed in Ref. [38] and first used in Refs. [39,40] in an experiment searching for parity (P) and time reversal invariance (T) violating electric dipole moment of xenon. Since then, this technique has been widely used in the experiments searching for P and T violating electric dipole moment in neutron [41,42], atoms [43–45], molecules [46,47], and solids [48].

In order to realize such a scanning strategy with a slope measuring instrument, the corresponding upgrade of the instrument should be made to allow automatic and simultaneous change of the orientation of a surface under test and the scanning direction of the profiler.

In the previous sections, we have discussed that the major contributions to the random and systematic errors of LTP measurements is significantly reduced by averaging over repeatable measurements performed with the SUT differently positioned in respect to the LTP. Above we have also shown that averaging over multiple scans performed according to the optimal scanning strategies with changing of the scanning direction and flipping of the SUT allows for significant reduction of the drift error. Therefore, with appropriate combinations of different SUT positions, orientations, and the LTP scanning directions, one can average out the major experimental errors of slope measurements with an LTP.

The ALS LTP-II and DLTP [14-16] already allow for automatic change of the scanning direction.

In the next Notes, we will describe the corresponding upgrade of the ALS LTP-II with an automated kinematic, rotational system that provides fully controlled flipping, tilting, and shifting of a SUT. The LTP-II equipped with the system is capable for simultaneous reversals of the scanning direction and the SUT orientation, and therefore, for complete realization of the advantages of the discussed method for suppression of errors in slope measurements.

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