

REPORT

An Uncertainty Budget

For the Metrological

Atomic Force Microscope

Jane Haycocks

September 2002

An Uncertainty Budget for the Metrological Atomic Force Microscope

Jane Haycocks

Centre for Basic, Thermal and Length Metrology

September 2002

ABSTRACT

The Metrological Atomic Force Microscope uses interferometry in three axes to deliver traceable dimensional measurements of standard samples. This report records the sources of uncertainty associated with the instrument, gives estimated values of these uncertainties and presents outline and example calculations of the combined measurement uncertainty for specific dimensional measurements of surface features. The uncertainty calculations follow the internationally accepted guidelines laid out in the Guide to the Expression of Uncertainty in Measurement.

© Crown Copyright 2002
Reproduced by Permission of the Controller of HMSO

ISSN 1469-4921

National Physical Laboratory
Queens Road, Teddington, Middlesex, TW11 0LW

No extracts from this report may be reproduced without the prior written consent of the Managing Director, National Physical Laboratory; if consent is given the source must be acknowledged and may not be used out of context.

Approved on behalf of the Managing Director, NPL
by Dr David Robinson, Head of Centre for Basic, Thermal and Length Metrology

Contents

1	Uncertainty analysis of the metrological AFM	2
1.1	Measurement process	2
1.2	Combined standard uncertainty	3
1.3	Mathematical model of the measurement	4
2	Standard uncertainties of input quantities	6
2.1	Interferometer data points	6
2.2	Vacuum frequency	7
2.3	Air refractive index	7
2.4	Cosine error	8
2.5	Orthogonality of the coordinate system	10
2.6	Abbe error	10
2.7	Dead path length uncertainty	11
2.8	Thermal expansion of the metrology frame	12
3	Summation of uncertainties	13
3.1	Special case: Step Height	13
3.2	Special case: Pitch measurement	14
4	Acknowledgements	15
5	References	15
6	Appendix 1: Sample calculations	17

Tables

Table 1	Uncertainties associated with x interferometer data	7
Table 2	Uncertainty in laser frequency	7
Table 3	Uncertainty in calculation of refractive index of air	8
Table 4	Estimated values of the angles contributing to cosine errors	10
Table 5	Estimated values of Abbe errors	11
Table 6	Estimated deadpath errors	11
Table 7	Estimated errors due to thermal expansion of the metrology frame	13

Figures

Figure 1:	Construction in Matlab for step height measurement	14
-----------	--	----

1 Uncertainty analysis of the metrological AFM

The uncertainty analysis of Metrological Atomic Force Microscope (MAFM) calculates the uncertainty of a length measurement made using optical interferometry on the x, y and z axes of the AFM. The uncertainty calculation follows internationally accepted guidelines for the evaluation and expression of uncertainties laid out in the Guide to the Expression of Uncertainty in Measurement (1995), referred to as the GUM.

1.1 Measurement process

The MAFM uses three optical interferometers to measure the relative displacement between the AFM tip and the sample. An x-y flexure stage scans the sample in discrete steps under the tip and data is recorded from the three interferometers at each step. The data is then be used to construct a 3D image of the surface of the sample with scales directly traceable to the national standard for length. Dimensional measurements of different surface features can be extracted.

The system control allows the operator to select options in the data collection process appropriate to the measurement task. Scan range, offset from the centre stage position and number of scan steps are independently variable in x and y, so any rectangular area within the range of the stage can be imaged with any number of pixels per line. The direction of the fast scan axis can be swapped between x and y; the x axis is the default selection. The time for data collection is dependent on the number of lines scanned and the number of pixels per line. Sources of uncertainty arising from fluctuations in ambient conditions are time-dependent so data collection time is an important consideration in the measurement strategy.

The raw spatial coordinate measurement data is imported into Matlab for analysis. The first stage is to apply a correction to the data to compensate for non-linearity in the interferometer response due to deviation of the two optical signals (sine and cosine) from perfect sinusoidal form (Heydemann 1981, Birch 1990). Thereafter the analysis depends on the desired measurement parameter. The main purpose of the MAFM is for calibration of transfer standards. Most standards are either 2 D grating structures for calibration of x and y scales, so the important measurands are x and/or y pitch, or step structures for calibration of z scales where the important measurand is step height. In general, there is little requirement for simultaneous measurement of relative heights and lateral dimensions on a sample.

As yet there are no internationally agreed specification standards on how calibration measurements should be made. For step heights a process that follows as closely as possible the method described for 2D profilometry in ISO 5436-1 (2000) has been adopted. The method defines the step height as the distance between 2 parallel straight lines fitted to specified upper and lower portions of the profile of a groove. The line fitting process involves statistical averaging of the data, so the uncertainty budget for the step height measurement will differ from the uncertainty budget for measurement of relative height between two data points.

1.2 Combined standard uncertainty

The first stage of the uncertainty analysis (GUM §4.1) is to establish a model equation for a measurand Y in terms of all the input quantities X_i .

$$Y = f(X_i). \quad (1)$$

An estimate, y , of the measurand, Y , is obtained from equation (1) using input estimates x_i for the values of X_i . The estimated standard deviation associated with the output estimate or the measurement result y , termed the combined standard uncertainty, $u_c(y)$, is determined from the estimated standard deviation associated with each input estimate x_i , termed the standard uncertainty $u(x_i)$. The combined standard uncertainty is the positive square root of the combined variance $u_c^2(y)$ which is given by (GUM §5.1)

$$u_c^2(y) = \sum_{i=1}^N \left[\frac{\partial f}{\partial x_i} \right]^2 u^2(x_i). \quad (2)$$

The partial derivatives are termed the sensitivity coefficients, usually denoted by c_i . Equation (2) may be rewritten as

$$u_c^2(y) = \sum_{i=1}^N [c_i u(x_i)]^2. \quad (3)$$

For the analysis of the MAFM system the input quantities are assumed to be uncorrelated, so no covariance terms have been included in equations (2) and (3).

The measurement uncertainties for MAFM measurements are generally expressed as expanded uncertainties. The expanded uncertainty U is defined as the combined uncertainty multiplied by a coverage factor k [§6.2 GUM],

$$U = ku_c(L) \quad (4)$$

Most measurements are expressed with a value of $k = 2$, corresponding to a confidence level of approximately 95%.

1.3 Mathematical model of the measurement

In this document the uncertainties associated with the following scenarios will be considered:

1) lateral separation of two points along one scan axis, L_x or L_y ; 2) lateral separation of two points anywhere on the scanned image L_{xy} ; 3) lateral separation of two points in the z axis L_z . The special cases of step height calculation and x -axis pitch are also considered.

1.3.1 Scenario 1

The measurand L_x is the difference between two data points in the x -axis when the x -axis has been selected as the fast scan direction. The model equation (equivalent to equation (1)) is

$$L_x = (x_2 - x_1) \frac{c}{4n\nu \cos\theta_a \cos\theta_m \cos\theta_t} + L_{Abbe} + L_{dp} + L_{mf} \quad (5)$$

where

x_1 and x_2 are two x -axis interferometer data points,

c is the vacuum speed of light,

n is the refractive index of air,

ν is the laser frequency,

θ_a is the angle between the measurement axis and the displacement axis,

θ_m is the angle between the incident laser beam and the mirror normal,

θ_t is the tilt angle of the sample relative to the x measurement axis,

L_{Abbe} is the correction factor for Abbe offset,

L_{dp} is the correction factor for the dead path length and

L_{mf} is the correction factor for thermal expansion in the metrology frame.

The sensitivity coefficients for insertion in equation (3) are:

$$c_{x_2} = \frac{\partial L_x}{\partial x_2} = \frac{c}{4vn \cos \theta_a \cos \theta_m \cos \theta_t} \quad (6)$$

$$c_{x_1} = \frac{\partial L_x}{\partial x_1} = \frac{-c}{4vn \cos \theta_a \cos \theta_m \cos \theta_t} \quad (7)$$

$$c_v = \frac{\partial L_x}{\partial v} = \frac{-(x_2 - x_1)c}{4v^2 n \cos \theta_a \cos \theta_m \cos \theta_t} \approx \frac{-L_x}{v} \quad (8)$$

$$c_n = \frac{\partial L_x}{\partial \mu} = \frac{-(x_2 - x_1)c}{4vn^2 \cos \theta_a \cos \theta_m \cos \theta_t} \approx \frac{-L_x}{n} \quad (9)$$

$$c_{\cos \theta_a} = \frac{\partial L_x}{\partial \cos \theta_a} = \frac{-(x_2 - x_1)c}{4vn \cos^2 \theta_a \cos \theta_m \cos \theta_t} \approx \frac{-L_x}{\cos \theta_a} \quad (10)$$

$$c_{\cos \theta_m} = \frac{\partial L_x}{\partial \cos \theta_m} = \frac{-(x_2 - x_1)c}{4vn \cos \theta_a \cos^2 \theta_m \cos \theta_t} \approx \frac{-L_x}{\cos \theta_m} \quad (11)$$

$$c_{\cos \theta_t} = \frac{\partial L_x}{\partial \cos \theta_t} = \frac{-(x_2 - x_1)c_t}{4vn \cos \theta_a \cos \theta_m \cos^2 \theta_t} \approx \frac{-L_x}{\cos \theta_t} \quad (12)$$

$$c_{L_{Abbe}} = \frac{\partial L_x}{\partial L_{Abbe}} = 1 \quad (13)$$

$$c_{L_{dp}} = \frac{\partial L_x}{\partial L_{dp}} = 1 \quad (14)$$

$$c_{L_{mf}} = \frac{\partial L_x}{\partial L_{mf}} = 1 \quad (15)$$

The mathematical analysis is the same for L_y but values for the estimated error contributions differ.

1.3.2 Scenario 2

The measurand L_{xy} is the difference between two data points (x_1, y_1) and (x_2, y_2) .

$$L_{xy} = (L_x^2 + L_y^2)^{\frac{1}{2}} (1 + \varepsilon) \quad (16)$$

where ε is the uncertainty due to non-orthogonality of the coordinate system. Partial derivatives give the sensitivity coefficients (assuming ε is small) as

$$c_{L_x} \approx \frac{L_x}{L_{xy}} \quad (17)$$

$$c_{L_y} \approx \frac{L_y}{L_{xy}} \quad (18)$$

$$c_{\varepsilon} \approx L_{xy} \quad (19)$$

The values for the estimated uncertainties in L_x and L_y differ from those in scenario 1 in the contribution for cosine error (discussed in section 2).

1.3.3 Scenario 3

For the measurand L_z , the separation between two data points in the z axis, the mathematical analysis is equivalent to that of scenario 1. However, usually z axis data is not used directly in this way. Normally, a best fit plane or best fit straight line would be extracted from the 3D or 2D data respectively to remove tilt from the image before relative heights of features are extracted. This fit also has the effect of compensating for approximately linear drifts in the system due to atmospheric changes. The estimates of the value of error contributions need to take into account the compensation effects of the data processing.

2 Standard uncertainties of the input quantities

2.1 Interferometer data points, x, y and z

The outputs of the interferometers are the integer number of optical fringes and the sine and cosine signal components. The uncertainty in the measurement of the integer number of optical fringes, N , is generally zero. For the fractional component (calculated from the sine and cosine signal components), the factors that determine uncertainty are: resolution of the counting system, linearity of response of the interferometers, and mechanical and electrical noise. The analogue outputs of the optical interferometers are converted to digital signals using an analogue-to-digital converter with a resolution of 4096 bits. However, the signals are usually adjusted to approximately three quarters of the full input range to avoid possible errors due to signal saturation. This gives a resolution of 0.0001 optical fringes. A Heydemann correction is applied to the data to correct for non-linearities in the interferometer response. The cyclic errors, which are evident on the uncorrected data, cannot be distinguished from the noise on the corrected data. Indeed a comparison of the optical interferometer with the NPL x-ray interferometer showed that cyclic errors on the Heydemann corrected data for an unstabilised laser source have amplitude of around 40 pm (Yacoot & Downs). This is well below the noise level on the interferometer data. Noise on the data may arise from the electronic detection system and mechanical oscillations. The overall rms noise is estimated be 0.005 fringes on the x and y axes data and 0.01 fringes on the z axis.

Source	Value / fringes	Divisor	Standard uncertainty / fringes	Sensitivity coefficient	Contribution / fringes
uncertainty in N	0	1	0	1	0
resolution of fringe counting cards	0.0001	$\sqrt{12}$	2.89×10^{-5}	1	2.89×10^{-5}
Rms noise	x/y 0.005 z 0.01	1	0.005 0.01	1	0.005 0.01
					x/y 0.005 z 0.01

Table 1 Uncertainties associated with x interferometer data

It should be noted that the summation above gives a value of the uncertainty of recording the interferometer data, but does not include uncertainties associated with the response of the AFM head. An assessment of the repeatability of the data points will include both the errors associated with response of the AFM head and the noise on the interferometer system.

2.2 Vacuum frequency, ν

The laser frequency of the three HeNe lasers used in the x, y and z axes interferometers were calibrated by beat frequency measurement against one of the standard NPL iodine-stabilised lasers. The frequencies of the three lasers were each measured as $473\,612\,700 \pm 700$ MHz.

Source	Value	Divisor	Standard uncertainty	Sensitivity coefficient	Contribution
Calibration uncertainty	± 700 MHz	2	± 350 MHz	1	350 MHz
					350 MHz

Table 2 Uncertainty in laser frequency

2.3 Air Refractive Index, n

The value for refractive index of air is calculated using the Edlen equation with corrections suggested by Birch & Downs (1994) and Bönsch and Potulski (1998). Standard conditions are assumed of temperature 20 °C, pressure 100 000 Pa, relative humidity of 50% and 0.04% carbon dioxide content. No subsequent correction is made for deviations away from these standard conditions. The laboratory has temperature control at $20 \pm 1^\circ\text{C}$, but local temperature rises near heat generating parts of the system (such as the lasers) can give $+2^\circ\text{C}$ temperature rise. Measurements of temperature, pressure and humidity have been taken over a period of time (several months) and the maximum deviations from standard conditions have been used in the estimate of uncertainty. The variation in carbon dioxide levels has not been measured; an estimate has been based on typical variations suggested by Downs (1998). Sensitivity coefficients for each variable have been calculated from the partial derivatives of the corrected Edlen equation.

Source	Value	divisor	Standard uncertainty	Sensitivity coefficient	Contribution
Temperature	2 °C	$\sqrt{3}$	1.155 °C	$9.20 \times 10^{-7}/^\circ\text{C}$	1.063×10^{-6}
Pressure	5000 Pa	$\sqrt{3}$	2886 Pa	$2.68 \times 10^{-9}/\text{Pa}$	7.734×10^{-6}
Humidity (partial pressure)	500 Pa	$\sqrt{3}$	289 Pa	$3.70 \times 10^{-10}/\text{Pa}$	1.069×10^{-7}
Carbon dioxide	100 ppm	$\sqrt{3}$	58 ppm	$1.4 \times 10^{-10}/\text{ppm}$	8.12×10^{-9}
Accuracy of Edlen equations	1×10^{-8}	1	1×10^{-8}	1	1×10^{-8}
					7.81×10^{-6}

Table 3 Uncertainty in calculation of refractive index of air

2.4 Cosine errors, θ_m , θ_a , θ_t

In an ideal configuration the interferometer beams would retroreflect perfectly from the target mirrors and the measurement axes should be aligned parallel to the directions of motion of the stage and the AFM head. For practical purposes the interferometers beams have been offset deliberately at a small angle from the retroreflected position to prevent light re-entering the laser tubes. This results

in a cosine error. The estimated angles of misalignment of the interferometer beams from the retroflected position, θ_m , is 2 mrad for all three axes.

For measurements extracted from data in two axis only (x/z or y/z) there will also be an error contribution from the misalignment of the measurement axis and the axis of motion. The estimated angles between the measurement axis and the motion axis, θ_a , are 2.2 mrad and 7.2 mrad for the x and y axes respectively in the x/y plane, measured by observing the displacement in the orthogonal axis as the flexure stage is scanned through its full range. The estimated angles between the z measurement axis and the z axis of motion are 0.1 rad in the x/z plane and 0.16 rad in the y/z plane. For three axes data there is no associated cosine error.

For step height measurements, single line data is often used. As the tip traverses the step in the x/z plane, there will be “cross-talk” motion in the y direction (of scale $z \tan \theta_a$ where z is the displacement in the z axis and θ_a is the angle of misalignment between the axes of motion and measurement). The tip will thus move along the groove in the y direction as it traverses in the x direction. The error in resultant step height measurement extracted from x/z data will be proportional to the tilt of the sample in the x/y plane. This tilt can be measured and the error can be corrected, provided the directions of the tilt and the direction of crosstalk movement are also measured. The estimated error for height measurement for uncorrected data is

$$\varepsilon = \tan \theta_a H \tan \theta_t \quad (20)$$

where θ_a is the angle between the measurement axis and direction of motion in the y/z plane, θ_t is the angle of tilt of the sample surface in the y direction with respect to the xy measurement plane, and H is the measured height. For a sample tilt of 10 mrad this gives error in measured height of $0.0016 H$ for single line measurements in the x scan direction. Equivalent analysis for scans in the y direction give an estimated error of $0.001 H$.

For x/y data in scenarios 1 and 2 there will be a cosine error associated with lateral measurement due to tilt of the sample. This could be corrected by using z axis data as well, but generally the sample tilt is small and line data in particular is often used without a correction for tilt. From observations of images of a selection of standard samples, the tilt is rarely greater than 10 mrad with respect to the x and y measurement axes.

Axis	Angles, mrad		
	θ_a	θ_m	θ_t
x	2.2 (x/y plane)	2	10
y	7.2 (x/y plane)	2	10
z	100 (x/z plane) 160 (y/z plane)	2	

Table 4 Estimated values of the angles contributing to cosine errors

2.5 Orthogonality of the coordinate system

Calculations of dimensions of surface features are made assuming an orthogonal co-ordinate system, i.e. it is assumed that the measurement axes of the three interferometers are orthogonal. The measurement axes of the interferometers are the normals to the reflecting faces of the target mirror blocks. The faces of the target mirror blocks are not perfectly orthogonal, so, consequently, an error is introduced into the calculations of dimensions. The deviations from orthogonality of the mirror blocks have been measured using a calibrated angle table and autocollimator.

The value of the error is dependent on both the length and the orientation of the measured dimension relative to the axes. The biggest error is along the diagonal of the co-ordinate system and is approximately 2 parts in 10^5 . For measurements that are approximately parallel to the x or y axes, the error is approximately 1 part in 10^5 .

2.6 Abbe error

The estimated offsets of the measurement axes from the point of interaction of the tip and sample are 3 mm for the x and y axes and 1 mm for the z axis. The angular errors of the x-y stage were measured using an angle interferometer. At a series of positions in x, the pitch, roll and yaw were measured as the stage was scanned in y. Similar measurements were made at y positions when the stage was scanned in x. The angular errors of the stage did not vary greatly as a function of position at which the scan was performed, and are approximately linear over the scan range. The angular errors in the AFM scan head for z axis motion were estimated using an autocollimator. Again the errors were approximately linear over the z axis range. The table below gives the estimated values of Abbe error for travel in the three axes, using a linear approximation of the angular errors and the estimated offsets.

Measurement axis	X-axis motion (stage) Error nm per μm travel	Y-axis motion (stage) Error nm per μm travel	Z-axis motion (head) Error nm per μm travel
X	0.12	-	3
Y	-	0.1	7.5
Z	0.068	0.046	2.7

Table 5 Estimated values of Abbe errors

2.7 Dead path length uncertainty

Dead path length, dp , is the difference in air-path length between the measurement and reference beams of the interferometer when the interferometer measurement is initiated. Dead path error occurs when there is a non-zero dead path and environmental conditions change during a measurement. The error is approximately

$$\varepsilon_{dp} = dp\Delta n \quad (21)$$

where Δn is the change in refractive index over the measurement time. For the MAFM interferometers, the effective dead path is the separation of the reflecting faces of the sample target mirror and the tip target mirror along the measurement axis. The dead path lengths are 10 mm in both the x and y axes, and 15 mm in the z-axes. The degree of variation of environmental conditions will be dependent on the measurement time. The table below shows estimated deadpath errors using the sensitivity coefficients of the Edlen equation quoted in table 3 above and typical measured values for changes in ambient conditions over the measurement time period.

Measurement axis	Error due to			
	Temperature change	Pressure change	Humidity change (partial pressure)	Quadrature Sum
X/Y	9.2 nm/°C	2.68 nm/mbar	3.7×10^{-3} nm/Pa	
Per pixel	3×10^{-5} nm	0.008 nm	0.03 nm	0.031 nm
Per 300 pixel line	0.009 nm	0.08 nm	0.03 nm	0.086 nm
Per 1000 pixel line	0.027 nm	0.08 nm	0.03 nm	0.090 nm
Per 5000 pixel line	0.12 nm	0.08 nm	0.03 nm	0.147 nm
Per 300 square image	2.39 nm	0.27 nm	0.03 nm	2.41 nm
Z	13.8 nm/°C	4.02 nm/mbar	0.0056 nm/Pa	
Per pixel	4×10^{-5} nm	0.012 nm	0.045 nm	0.047 nm
Per 300 pixel line	0.014 nm	0.12 nm	0.045 nm	0.129 nm
Per 1000 pixel line	0.041 nm	0.12 nm	0.045 nm	0.135 nm
Per 5000 pixel line	0.18 nm	0.12 nm	0.045 nm	0.221 nm
Per 300 square image	3.6 nm	0.4 nm	0.045 nm	3.62 nm

Table 6 Estimated deadpath errors

2.8 Thermal expansion of the metrology frame

Thermal expansion of the components of the metrology frame will result in net displacements in the positions of the AFM tip and sample. Since the interferometers measure relative displacements between the tip and the sample, no error is incurred due to thermal expansion of components in the bulk metrology frame. However, a small error will be incurred due to the thermal expansion of interfacing components between the tip target mirror and the tip and between the sample target mirror and the sample, and due to thermal expansion of the mirrors themselves.

The sample is mounted on a magnet glued to a stainless steel holder. The sample holder is circular in shape and is mounted kinematically on three radial grooves that locate onto three balls attached to the mirror block. The point of interaction between the tip and sample is designed to be close to the centre of the sample holder. Any thermal expansion of the sample holder in the x/y plane should occur radially, with negligible shift in the lateral position of the sample. The mirror block itself is mounted onto the stage in a similar way so thermal expansion of the mirror base should produce negligible shift in the lateral position of centre point of the 3 balls with respect to the AFM tip. However thermal expansion of the mirror blocks displaces the target mirrors with respect to the lateral sample/tip positions. In the z-axis, thermal expansion of the mirror, the components of the sample holder and the sample itself will result in a net displacement of the sample with respect to the sample target mirror surface.

The AFM cantilever protrudes from a silicon base of approximate dimensions 4 mm x 1.5 mm x 0.5 mm, which is glued to a steel bar. Since the cantilever is glued firmly to the steel bar, this assembly is likely bend like a bimetallic strip under thermal fluctuations. The steel bar is held magnetically in a groove on an aluminium holder attached to the scan tube. The holder is designed to place the tip close to the centre of the scan tube. Thermal expansion of the aluminium holder is assumed to be radial and will shift the position of the groove that holds the cantilever away from the centre (along the x-axis). The tip target mirror is glued to the aluminium holder. It is assumed that the mirror will expand laterally giving a net displacement of the mirror surface from the tip position in x and y. In the z-axis it is assumed that the tip mirror surface will track thermal expansion changes in the aluminium holder (which assumes that they are attached together at the lower face of the holder). It is also assumed that the mirror can expand in z, unconstrained by the glued interface to the aluminium holder at the corners where the z-axis measurement beams are reflected.

Estimates of the error arising from net displacement due to thermal expansion of measured position from true position are given in the table below. These have been calculated using measured values of temperature fluctuations over the time period of the AFM measurement. In the z axis, the effect of a drift in temperature at an approximately constant rate over the measurement period will be indistinguishable from the effect of tilt on the sample. A best fit plane is usually extracted from the data to remove tilt before making z dimensional measurements; this will compensate for the effects of linear drift in temperature.

Error	X axis / nm	Y axis / nm	Z axis / nm
Per °C change	5.8	17.2	62.2
Per pixel	1.7×10^{-5}	5.1×10^{-5}	1.89×10^{-4}
Per 300 pixel line	5.8×10^{-3}	0.017	0.062
Per 1000 pixel line	0.017	0.052	0.187
Per 5000 pixel line	0.08	0.22	0.81
Per 300 square image	1.4	4.5	16.2

Table 7: Estimated errors due to thermal expansion of the metrology frame

3 Summation of uncertainties

An error budget for any particular measurement may be calculated from appropriate summation of the estimated values of the individual contributions given in the previous section. Outline budgets for the three scenarios listed at section one have been constructed in Excel and sample calculations are attached at Appendix 1.

3.1 Special case: Step Height

In section 1 it was noted that step height measurements are made following as closely as possible the method given for 2D profilometry in ISO 5436. The analysis is carried out using Matlab and Figure 1 shows the construction made to calculate the step height. In section 2 error contributions for step height measurement that differ from those for a measurement of L_z were noted. The step height H is given by

$$H = h \frac{c \cos \theta_t}{4n \nu \cos \theta_m} + L_{Abbe} + L_{dp} + L_{mf} + L_{ct}, \quad (22)$$

where h is the separation in fringes in the z axis of the two parallel lines fitted to the upper and lower sections of the step in the construction in Figure 1, L_{ct} is the correction factor for the

crosstalk movement of the AFM tip along the step described in section 2.4, and all other parameters are as defined in section 1.3.1. The value of h is the difference in the intercepts of the two fitted parallel lines; the $\cos\theta_i$ term on the top line effectively converts this into the perpendicular distance between the two lines. The uncertainty associated with h includes both the uncertainty associated with the data processing method and the uncertainty associated with the data. The latter is a combination of the factors noted at section 2.1 and the repeatability of the measurement.

An example spreadsheet calculation of the step height uncertainty is included in Appendix 1.

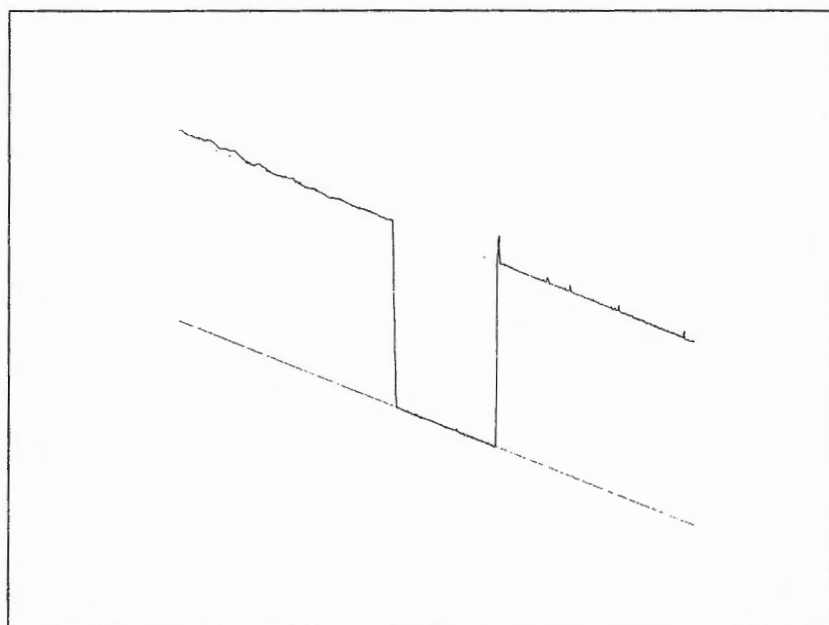


Figure 1: Construction in Matlab for step height measurement

3.2 Special case: Pitch measurement

There is no agreed standard method for extracting pitch measurement from SPM data. For the MAFM (in common with most SPMs) the errors associated with the fast scan direction are smaller than the slow scan direction, so pitch measurement would usually be made using predominantly fast scan axis data. As yet a routine method for pitch measurement has not been established for the MAFM, as samples that have been examined to date vary significantly in pitch, profile and uniformity. So far pitch has been extracted from MAFM data either by using a cursor to select data points on a 3D image or 2D profile, or by using fitting algorithms on 2D data to identify peaks for sinusoidal grating profiles or intercepts with a straight line for sinusoidal or other profiles.

For 2D data the analysis in scenario 1, section 1.3.1, applies, but an additional correction factor is added to compensate for the misalignment between the grating lines and the perpendicular direction to the scan. The pitch P is given by

$$P = p \frac{c \cos \theta_g}{4n\nu \cos \theta_a \cos \theta_m \cos \theta_t} + L_{Abbe} + L_{dp} + L_{mf} \quad (23)$$

where p is the value in fringes for pitch extract from the data, θ_g is the angle between the grating lines and the perpendicular to the scan direction (estimated from a 3D image of the sample) and all other parameters are as defined in section 1.3.1. The uncertainty associated with p includes the repeatability of the data and the uncertainty associated with the processing method.

For 3D data the mathematical analysis in scenario 2, section 1.3.2 applies. The uncertainties associated with the data points must include those associated with repeatability and those associated with the data processing method.

4 Acknowledgements

The format for this uncertainty analysis is based on the approach used for presentation of measurement uncertainty for the NPL Nanosurf IV instrument (Leach). This work was funded by the DTI NMS Length Programme 1999 – 2002 project LE9952.

5 References

- PD 6461 1995 Part 3 Guide to the expression of uncertainty in measurement, published by BSI, London
- Bönsch G, Potulski E 1998 Measurement of the refractive index of air and comparison with the Edlén formulae *Metrologia* **10** 137-143
- Birch K P 1990 Optical fringe subdivision with nanometric accuracy *Prec. Eng.* **12** 195-198
- Birch K P, & Downs MJ 1994 Correction to the updated Edlén equation for the refractive index of air *Metrologia* **31** 315-316
- Downs M J 1998 Realisation of the optimum performance from length measuring interferometers by atmospheric refractometry *Proc. SPIE* **3477** 46-53
- Heydemann P L M 1981 Determination and correction of quadrature fringe measurement errors in interferometers *Appl. Opt.* **20** 3382-4

ISO 5436-1 2000 Geometrical Product Specifications (GPS) – Surface texture: Profile method; Measurement standards – Part 1: Material measures

Leach R K 1999 Calibration, traceability and uncertainty issues in surface texture metrology *NPL Report CLM 7*

Yacoot A & Downs M J 2000 The use of x-ray interferometry to investigate the linearity of the NPL differential Plane Mirror Optical Interferometer *Meas. Sci. Technol.* **11** 1126-1130

Appendix 1: Sample Calculations

A1: Lateral separation of 2 points along the fast scan axis

The attached sheets show the summation of uncertainties for measurement of the separation between two points in the fast scan axis when x is the fast scan direction (A1.1) and when y is the fast scan direction (A1.2). The values for Abbe error, cosine alignment error and thermal drift in the metrology frame differ between the two axes, but the data point uncertainty is dominant. This uncertainty arises from noise (both mechanical and electronic). A measurement of a lateral dimension would usually be the mean of a number of repeated measurements, so the noise would be reduced by averaging. The uncertainty associated with the data points would be replaced in the calculation by the error of the mean.

A1.1a shows the uncertainty calculated with a data point separation of zero in the x axis, which gives a baseline estimate of 1.1 nm on the measurement uncertainty. A1.1b, c and d show the calculations for 1 nm, 1 μm and 100 μm respectively. The uncertainty continues to be dominated by the noise on the individual data points up to lengths around 1 μm . Then as the dimensions increase the length dependent uncertainties have more significant effect. A1.2 gives the uncertainty for the y axis as the fast scan axis for a zero data point separation. The difference in the combined uncertainties for the x and y scan axes is negligible for zero and sub μm dimensions; as dimensions increase above 1 μm the differences begin to become significant as the length dependent uncertainties begin to dominate. It should be noted that if the uncertainty associated with the data points is reduced by using averaged values, then the length dependent uncertainties will be significant at lengths less than 1 μm .

A2: Lateral separation of 2 points in x/y

The attached sheet A2 shows the calculation of the combined uncertainty for a measurement of the separation of two points on an image of 300 x 300 pixels and 100 x 100 μm ranges. The two points selected were opposite corners of the image. The uncertainties associated with the separation of the data points in x and in y were calculated using the spreadsheets shown in A1 but with the cosine error associated with axes alignment $\cos \theta_a$ excluded.

A3: Special case – step height

The attached sheet A3 shows the calculation of the corrected step height, combined and expanded uncertainty (95% confidence limit) of a standard sample (identified as H24). Five repeat line scans

were made and analysed at 5 locations, separated by a few micrometres across the length of the step, at 4 separately identified reference areas. The step height for each scanned location was calculated as the averaged value from the 5 repeat lines. The value used for step height h on the spreadsheet was the average value of the 5 scans at the 4 reference areas (20 values) and the uncertainty in h is the standard uncertainty of the mean. It is notable that the averaging of the measurements has delivered a significant decrease in the uncertainty associated with individual z axis data points.

A1.1a Lateral separation of 2 points along the x scan axis

$$L_x = (x_2 - x_1) \frac{c}{4nV \cos\theta_a \cos\theta_m \cos\theta_l} + L_{abbe} + L_{tip} + L_{mf} \quad Lx = \quad 0 \text{ m}$$

c = speed of light in vacuum : 299792458

quantity	estimate	uncertainty units	probability sensitivity distribution coeff	uncertainty contribution (m)	degrees of freedom
data point x_1	0	0.005 fringes	1.5821E-07	7.91E-10	7.9103E-10 > 100
data point x_2	0	0.005 fringes	1.5821E-07	7.91E-10	7.9103E-10 > 100
refractive index of air n	1.000268	7.81E-06	0.99973207 L	7.81E-06 L	0.00E+00 inf
laser frequency V	4.7361E+14	3.50E+08 Hz	2.1114E-15 L	7.39E-07 L	0.00E+00 inf
cosine error angle, $\cos\theta_a$	1	2.42E-06	1.00000242 L	1.40E-06 L	0.00E+00 inf
cosine error angle, $\cos\theta_m$	1	2.00E-06	1.000002 L	1.15E-06 L	0.00E+00 inf
sample tilt angle, $\cos\theta_l$	1	5.00E-05	1.00005 L	2.89E-05 L	0.00E+00 inf
Abbe correction L_{abbe}	0	1.20E-04 m	L	6.93E-05 L	0.00E+00 inf
Dead path correction L_{tip}	0	3.10E-02 nm per pixel	R	1.79E-11	1.79E-11 inf
		8.60E-02 nm over 300 pixels		4.97E-11	4.97E-11 inf
		9.00E-02 nm over 1000 pixels		5.20E-11	5.20E-11 inf
		1.57E-01 nm over 5000 pixels		9.06E-11	9.06E-11 inf
Metrology frame correction L_{mf}	0	1.70E-05 nm per pixel	R	9.81E-15	9.81E-15 inf
		5.80E-03 nm over 300 pixels		3.35E-12	3.35E-12 inf
		1.70E-02 nm over 1000 pixels		9.81E-12	9.81E-12 inf
		8.00E-02 nm over 5000 pixels		4.62E-11	4.62E-11 inf
		quadrature sum per pixel	sqrt	1.252E-18 +	5.698E-09 L*L = 1.119E-09
		nm over 300 pixels	sqrt	1.254E-18 +	5.698E-09 L*L = 1.120E-09
		nm over 1000 pixels	sqrt	1.254E-18 +	5.698E-09 L*L = 1.120E-09
		nm over 5000 pixels	sqrt	1.262E-18 +	5.698E-09 L*L = 1.123E-09

A1.1b Lateral separation of 2 points along the x scan axis

$$L_x = (x_2 - x_1) \frac{c}{4nV \cos\theta_a \cos\theta_m \cos\theta_i} + L_{abbe} + L_{dp} + L_{mf} \quad Lx = 1E-09 \text{ m}$$

c = speed of light in vacuum = 299792458

quantity	estimate	uncertainty units	probability distribution	sensitivity coeff	uncertainty contribution (m)	degrees of freedom
data point x_1	0	0.005 fringes	N	1.5821E-07	7.91E-10	7.9103E-10 >100
data point x_2	0.006321	0.005 fringes	N	1.5821E-07	7.91E-10	7.9103E-10 >100
refractive index of air n	1.000268	7.81E-06	N	0.99973207	7.81E-06	7.81E-15 inf
laser frequency V	4.7361E+14	3.50E+08 Hz	N	2.1114E-15	7.39E-07	7.39E-16 inf
cosine error angle, $\cos\theta_a$	1	2.42E-06	R	1.00000242	1.40E-06	1.40E-15 inf
cosine error angle, $\cos\theta_m$	1	2.00E-06	R	1.000002	1.15E-06	1.15E-15 inf
sample tilt angle, $\cos\theta_i$	1	5.00E-05	R	1.00005	2.89E-05	2.89E-14 inf
Abbe correction L_{abbe}	0	1.20E-04 m	R		6.93E-05	6.93E-14 inf
Dead path correction L_{dp}	0	3.10E-02 nm per pixel	R	1	1.79E-11	1.79E-11 inf
		8.60E-02 nm over 300 pixels			4.97E-11	4.97E-11 inf
		9.00E-02 nm over 1000 pixels			5.20E-11	5.20E-11 inf
		1.57E-01 nm over 5000 pixels			9.06E-11	9.06E-11 inf
Metrology frame correction L_{mf}	0	1.70E-05 nm per pixel	R	1	9.81E-15	9.81E-15 inf
		5.80E-03 nm over 300 pixels			3.35E-12	3.35E-12 inf
		1.70E-02 nm over 1000 pixels			9.81E-12	9.81E-12 inf
		8.00E-02 nm over 5000 pixels			4.62E-11	4.62E-11 inf
quadrature si nm per pixel						
		nm over 300 pixels		sqrt	1.252E-18 +	5.698E-09 L*L = 1.119E-09
		nm over 1000 pixels		sqrt	1.254E-18 +	5.698E-09 L*L = 1.120E-09
		nm over 5000 pixels		sqrt	1.254E-18 +	5.698E-09 L*L = 1.120E-09
		nm over 5000 pixels		sqrt	1.262E-18 +	5.698E-09 L*L = 1.123E-09

A1.1c Lateral separation of 2 points along the x scan axis

$$L_x = (x_2 - x_1) \frac{c}{4nv \cos \theta_a \cos \theta_m \cos \theta_t} + L_{abbe} + L_{dp} + L_{mf} \quad Lx = 1E-06 \text{ m}$$

c = speed of light in vacuum : 299792458

quantity	estimate	uncertainty units	probability distribution	sensitivity coeff	uncertainty contribution (m)	degrees of freedom
data point x_1	0	0.005 fringes	N	1.5821E-07	7.91E-10	7.9103E-10 >100
data point x_2	6.321	0.005 fringes	N	1.5821E-07	7.91E-10	7.9103E-10 >100
refractive index of air n	1.000268	7.81E-06	N	0.99973207	7.81E-06 L	7.81E-12 inf
laser frequency V	4.7361E+14	3.50E+08 Hz	N	2.1114E-15	7.39E-07 L	7.39E-13 inf
cosine error angle, $\cos \theta_a$	1	2.42E-06	R	1.00000242	1.40E-06 L	1.40E-12 inf
cosine error angle, $\cos \theta_m$	1	2.00E-06	R	1.000002	1.15E-06 L	1.15E-12 inf
sample tilt angle, $\cos \theta_t$	1	5.00E-05	R	1.00005	2.89E-05 L	2.89E-11 inf
Abbe correction L_{abbe}	0	1.20E-04 m	R	L	6.93E-05 L	6.93E-11 inf
Dead path correction L_{dp}	0	3.10E-02 nm per pixel	R	1	1.79E-11	1.79E-11 inf
		8.60E-02 nm over 300 pixels			4.97E-11	4.97E-11 inf
		9.00E-02 nm over 1000 pixels			5.20E-11	5.20E-11 inf
		1.57E-01 nm over 5000 pixels			9.06E-11	9.06E-11 inf
Metrology frame correction L_{mf}	0	1.70E-05 nm per pixel	R	1	9.81E-15	9.81E-15 inf
		5.80E-03 nm over 300 pixels			3.35E-12	3.35E-12 inf
		1.70E-02 nm over 1000 pixels			9.81E-12	9.81E-12 inf
		8.00E-02 nm over 5000 pixels			4.62E-11	4.62E-11 inf
		quadrature sum				
		nm per pixel			sqrt 1.252E-18 +	5.698E-09 L*L = 1.121E-09
		nm over 300 pixels			sqrt 1.254E-18 +	5.698E-09 L*L = 1.122E-09
		nm over 1000 pixels			sqrt 1.254E-18 +	5.698E-09 L*L = 1.122E-09
		nm over 5000 pixels			sqrt 1.262E-18 +	5.698E-09 L*L = 1.126E-09

A1.1d Lateral separation of 2 points along the x scan axis

$$L_x = (x_2 - x_1) \frac{c}{4nV \cos \theta_a \cos \theta_m \cos \theta_i} + L_{abbe} + L_{dp} + L_{mf} \quad Lx = \quad 0.0001 \text{ m}$$

c = speed of light in vacuum = 299792458

quantity	estimate	uncertainty units	probability sensitivity distribution coeff	uncertainty contribution (m)	degrees of freedom
data point x_1	0	0.005 fringes	1.5821E-07	7.91E-10	7.9103E-10 >100
data point x_2	632.1	0.005 fringes	1.5821E-07	7.91E-10	7.9103E-10 >100
refractive index of air n	1.000268	7.81E-06	0.99973207 L	7.81E-06 L	7.81E-10 inf
laser frequency V	4.7361E+14	3.50E+08 Hz	2.1114E-15 L	7.39E-07 L	7.39E-11 inf
cosine error angle, $\cos \theta_a$	1	2.42E-06	1.00000242 L	1.40E-06 L	1.40E-10 inf
cosine error angle, $\cos \theta_m$	1	2.00E-06	1.000002 L	1.15E-06 L	1.15E-10 inf
sample tilt angle, $\cos \theta_i$	1	5.00E-05	1.00005 L	2.89E-05 L	2.89E-09 inf
Abbe correction L_{abbe}	0	1.20E-04 m	L	6.93E-05 L	6.93E-09 inf
Dead path correction L_{dp}	0	3.10E-02 nm per pixel	1	1.79E-11	1.79E-11 inf
		8.60E-02 nm over 300 pixels		4.97E-11	4.97E-11 inf
		9.00E-02 nm over 1000 pixels		5.20E-11	5.20E-11 inf
		1.57E-01 nm over 5000 pixels		9.06E-11	9.06E-11 inf
Metrology frame correction L_{mf}	0	1.70E-05 nm per pixel	1	9.81E-15	9.81E-15 inf
		5.80E-03 nm over 300 pixels		3.35E-12	3.35E-12 inf
		1.70E-02 nm over 1000 pixels		9.81E-12	9.81E-12 inf
		8.00E-02 nm over 5000 pixels		4.62E-11	4.62E-11 inf
		quadrature st nm per pixel			
		nm over 300 pixels	sqrt	1.252E-18 +	5.698E-09 L*L = 7.631E-09
		nm over 1000 pixels	sqrt	1.254E-18 +	5.698E-09 L*L = 7.631E-09
		nm over 5000 pixels	sqrt	1.254E-18 +	5.698E-09 L*L = 7.631E-09
		nm over 5000 pixels	sqrt	1.262E-18 +	5.698E-09 L*L = 7.632E-09

A1.2: Lateral separation of 2 points along the y scan axis

$$L_y = (y_2 - y_1) \frac{c}{4nV \cos \theta_a \cos \theta_m \cos \theta_i} + L_{abbe} + L_{dp} + L_{mf}$$

c = speed of light in vacuum = 299792458

Ly= 0 m

quantity	estimate	uncertainty units	probability sensitivity distribution coeff	uncertainty contribution (m)	degrees of freedom
data point y_1	0	0.005 fringes	1.5821E-07	7.910E-10	7.910E-10 > 100
data point y_2	0	0.005 fringes	1.5821E-07	7.910E-10	7.910E-10 > 100
refractive index of air n	1.000268	7.81E-06	0.99973207	7.808E-06	0.000E+00 inf
laser frequency V	4.7361E+14	3.50E+08 Hz	2.1114E-15	7.390E-07	0.000E+00 inf
cosine error angle, $\cos \theta_a$	1	2.59E-05	1.00002592	1.497E-05	0.000E+00 inf
cosine error angle, $\cos \theta_m$	1	2.00E-06	1.000002	1.155E-06	0.000E+00 inf
sample tilt angle, $\cos \theta_i$	1	5.00E-05	1.00005	2.887E-05	0.000E+00 inf
Abbe correction L_{abbe}	0	1.00E-04 m		5.774E-05	0.000E+00 inf
Dead path correction L_{dp}	0	3.10E-02 nm per pixel	1	1.790E-11	1.790E-11 inf
		8.60E-02 nm over 300 pixels		4.965E-11	4.965E-11 inf
		9.00E-02 nm over 1000 pixels		5.196E-11	5.196E-11 inf
		1.57E-01 nm over 5000 pixels		9.064E-11	9.064E-11 inf
Metrology frame correction L_{mf}	0	5.10E-05 nm per pixel	1	2.944E-14	2.944E-14 inf
		1.70E-02 nm over 300 pixels		9.815E-12	9.815E-12 inf
		5.20E-02 nm over 1000 pixels		3.002E-11	3.002E-11 inf
		2.20E-01 nm over 5000 pixels		1.270E-10	1.270E-10 inf
	quad sum				
	per pixel			1.252E-18	4.454E-09 $L^*L =$
	300 pixel line			1.254E-18	4.454E-09 $L^*L =$
	1000 pixel line			1.255E-18	4.454E-09 $L^*L =$
	5000 pixel line			1.276E-18	4.454E-09 $L^*L =$
					1.119E-09
					1.120E-09
					1.120E-09
					1.130E-09

A2.1 Lateral separation of 2 points in x/y

$$L_{xy} = (L_x^2 + L_y^2)^{\frac{1}{2}} (1 + \epsilon)$$

$$= 1.414\text{E-}04 \text{ m}$$

quantity	estimate	uncertainty	units	probability distribution	sensitivity coeff	uncertainty contribution	degrees of freedom
Lx	1.000E-04	7.798E-09	m	N	0.707107	5.51385E-09	>100
Ly	1.000E-04	7.227E-09	m	N	0.707107	5.11051E-09	>100
E	0	0.00002		R	0.000141	1.63302E-09	inf
Quadrature sum						7.69328E-09	

A3: Special case - step heights		sample id	H24						
$L = h \frac{c \cos \theta_t}{4nV \cos \theta_m} + L_{abbe} + L_{dp} + L_{mf} + L_{ct}$									
$c = \text{speed of light in vacuum} =$				299792458					
quantity	estimate	uncertainty	units	probability distribution	sensitivity coeff	uncertainty contribution (m)	sq of uncertainty contribution	dof	
Step height h	0.08783	0.00041	fringes	N	1.58205E-07	6.486E-11	6.486E-11	19	
refractive index of air n	1.000268	7.81E-06		N	0.999732072	7.808E-06 L	6.858E-16	inf	
laser frequency V	4.7361E+14	3.50E+08	Hz	N	2.11143E-15	7.390E-07 L	6.491E-17	inf	
cosine error angle, $\cos \theta_t$	1	2.00E-06		R	1.000002	1.155E-06 L	1.014E-16	inf	
sample tilt angle, $\cos \theta_m$	1	2.50E-06		R	3E-05	4.330E-11 L	3.803E-21	inf	
Abbe correction L_{abbe}	0	2.70E-03	m	R		1.559E-03 L	1.369E-13	inf	
Dead path correction L_{dp}	0	1.35E-01	nm	R	1	7.794E-11	7.794E-11	inf	
Metrology frame correction L_{mf}	0	1.87E-01	nm	R	1	1.080E-10	1.080E-10	inf	
Cross talk correction L_{ct}	0	2.551E-06		R	1	1.473E-15	1.473E-15	inf	
						sum	2.194E-20		
						sqrt	1.481E-10		
						effective dof =	2.918E+43		
				step height L in metres =	1.390E-08				
				expanded uncertainty, $k = 2$	2.962E-10				