

Algorithms to evaluate spherical depth standards for optical form interferometry

Dorothee Hüser, Markus Schake, Gerd Ehret

Physikalisch-Technische Bundesanstalt, Braunschweig, Germany

September 2026

1 The Software

The Python programs `ana_DS_calib.py`, implementing the calibration procedure, and `ana_DS_study.py`, for investigating the influence of variations in the evaluation parameters, both call the algorithms described in Section 2, which are collected in the module `algos_DSana.py`.

The program `ana_DS_calib.py` processes all data files in a user-selected directory that match a user-defined filename pattern. For each data set, it generates a map of the evaluation regions together with a profile view containing four representative cross sections. These profiles illustrate the form deviation of the reference plateau but are not used in the areal depth evaluation.

The repository contains four example data sets acquired at the rotational orientations 0° , 90° , 180° , and 270° , obtained by rotating the depth standard about the optical axis (see Fig. 1).

2 Areal and radial-profile evaluation of a spherical cap

In flatness metrology, the field of view typically spans several tens to several hundreds of millimetres. Consequently, the 25.4 mm depth standard occupies only a small fraction of the camera field and is mounted in the rotatable holder shown in Fig. 1.

For further processing, a rectangular subaperture enclosing the measurement object is cropped

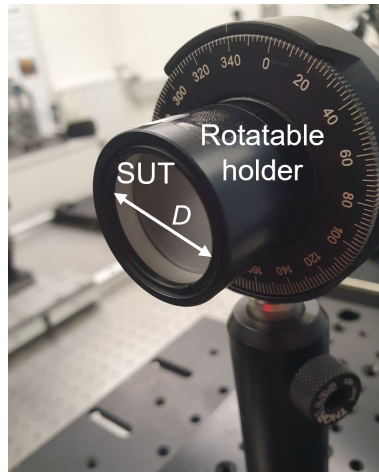


Figure 1: Surface under test (SUT) mounted in a rotatable holder.

from the measured topography. Pixels outside the circular object boundary are assigned *not-a-number* (NaN) values. Missing values inside the object boundary are interpolated solely for the segmentation steps used to distinguish the spherical cap from the reference plateau. These interpolated values are excluded from all subsequent quantitative evaluations, in particular from the least-squares fits of the reference plane and the spherical cap.

```

1 # Within the circular area representing the object surface ,
2 # remaining invalid data points are replaced by interpolated values
3 # to facilitate segmentation algorithms conveniently; more stable
4 z_map_um = algos_DSana.fill_nan_inside_circle(z_map_um_raw)
5 valid_fit = (
6     np.invert(np.isnan(z_map_um_raw))
7     & np.invert(np.isnan(z_map_um))
8 )

```

The two main programs, `ana_DS_calib.py` and `ana_DS_study.py`, each contain a main function, `analyse_depth()`, implementing the respective evaluation workflow. In both programs, the data processing is performed with the following steps:

Step 1: Rough estimate of the sphere cap center

In a first step, a coarse estimate of the lateral coordinates of the cap centre, $(x_{c,circ}, y_{c,circ})$, is obtained by fitting a circular disk of radius r_{circ} to the central region of the cap. The set of indices corresponding to the data points located within the circular region is denoted by I_{circ} .

This is called by `analyse_depth` with

```

1 # determination of index set of the circular disk
2 #
3 (
4     i_sph_1st ,
5     pcirc_um ,
6     x_gridum , y_gridum
7 ) = analyse_edgetrans(dx_um, dy_um, z_map_um)

```

The data points associated with the maximum slope are selected for the circular fit. In accordance with ISO 25178-2 and ISO 21920-2 the slopes are determined from local gradients based on sixth-degree local polynomials. The function `analyse_edgetrans` is located in the main modules `ana_DS_calib.py` and `ana_DS_study.py` calling

```

1 # determine the index set of the circular disk
2 # of the region for the cap fitting
3 (
4     x_c_um , y_c_um ,
5     radius_um ,
6     i_disk , _
7 ) = algos_DSana.determine_capdisk(
8     x_gridum , y_gridum , z_map_um
9 )

```

where the gradient based circle detection is performed. In `determine_capdisk` of module `algos_DSana` this is

```

1 # evaluate gradient and curvature according to
2 # Annex D.1 for the gradient and D.2 for the curvature ,
3 # of the ISO standard , here , the gradient is used
4 d_x = x_gridum[0][1] - x_gridum[0][0]
5 d_y = y_gridum[1][0] - y_gridum[0][0]
6 z_grad , _ = grad_curv(d_x, d_y, z_map_um)
7 iuse = np.where(np.invert(np.isnan(z_grad)))

```

The threshold to define the steepest decent is estimated using `find_peaks` from `scipy.signal`

```

1 # determination of the threshold value to define
2 # steepest slopes
3 hist, bin_edges = np.histogram(z_grad[iuse], bins=100)
4 z_bins = 0.5 * (bin_edges[1:101] + bin_edges[0:100])
5
6 idx_peak, _ = find_peaks(np.abs(hist), height=0)
7 idx_sh = np.argsort(hist[idx_peak])[::-1]
8
9 z_upper = np.max(z_bins[idx_peak[idx_sh[0:2]]])
10 z_mid = np.mean(z_bins[idx_peak[idx_sh[0:2]]])
11 idx_upperpeak = np.where(z_bins > z_mid)[0]
12
13 weights = hist[idx_upperpeak]
14 deviation = z_bins[idx_upperpeak] - z_upper
15
16 peak_width = np.sqrt(
17     np.sum(weights * deviation**2)
18     / np.sum(weights)
19 )
20 zg_thr = z_upper - peak_width

```

The resulting circle parameters are then used as initial values for fitting a radially symmetric paraboloid to the data points within the central cap region, i.e. with indices in I_{circ} . The paraboloid model is given by

$$z_{\text{cap}}(\mathbf{p}, x, y) = \frac{1}{2p_2} ((x - p_0)^2 + (y - p_1)^2) + p_3, \quad \mathbf{p} = (p_0, p_1, p_2, p_3)^T, \quad (1)$$

where (p_0, p_1) are the lateral centre coordinates, p_2 is the signed radius of curvature at the vertex, and p_3 is the vertex height.

A paraboloid is used instead of the exact spherical sag equation because it gives a well-conditioned fit whose parameters have a direct geometric interpretation. For the present standards, the sag-to-aperture ratio is of order 10^{-4} , and the quartic correction that distinguishes a sphere from its paraxial paraboloid is negligible over the central fitting region.

The centre coordinates obtained from the parabolic fit in this first processing step, $(p_0, p_1) = (x_{\text{c,step 1}}, y_{\text{c,step 1}})$, form the basis for the subsequent refinement of the determination of the transition region between the spherical cap and the reference plateau.

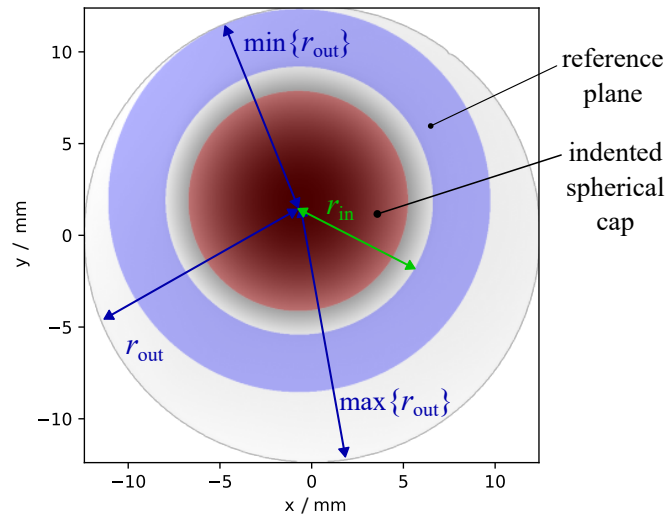


Figure 2: Segmentation of the regions for fitting the reference plane and the spherical cap; as the spherical cap is eccentrically embedded on the object, the reference-plane region forms a complete annulus only for $r_{\text{out}} \leq \min\{r(\varphi)\}$.

This is called by `analyse_depth` with

```

1 # for a more precise detection of the cap center
2 #
3 dr_um = np.sqrt(dx_um**2 + dy_um**2)
4 mask_sph_1st = np.zeros_like(valid_fit, dtype=bool)
5 mask_sph_1st[i_sph_1st] = True
6 i_sph_1st_fit = np.where(mask_sph_1st & valid_fit)
7 (
8     psphere_um,
9     sigma_pshp, covar_sph, sigma_resisph_um
10 ) = algos_DSana.fit_parabo(
11     x_gridum[i_sph_1st_fit].flatten(),
12     y_gridum[i_sph_1st_fit].flatten(),
13     z_map_um[i_sph_1st_fit].flatten(),
14     dr_um, pcirc_um
15 )

```

A challenge associated with the sphere cap measurement objects is that the reference plateau exhibits form deviations on the order of $0.1 \mu\text{m}$, corresponding to approximately 10 % of the spherical cap depth. The form deviations may arise from the polishing process. Deterministic polishing acts through a finite tool influence function. Near edges or boundaries, the

pressure-removal distribution changes and produces edge effects such as roll-off or turned edges. Therefore, in a 25 mm quartz disk with a 20 mm cap diameter and only a 2.5 mm surrounding annulus, maintaining that annulus perfectly flat is a manufacturing challenge. An annular deformation of around $0.1 \mu\text{m}$ could be explained by known edge effects in optical polishing.

These deviations introduce a bias in the determination of the transition between the spherical cap and the planar reference region and lead to a dependence of the evaluated depth on the size of the selected reference area on the plateau.

Step 2: Improved estimate of the sphere cap center

Therefore, in the second step, in case of `ana_DS_study.py` a set of reference regions is defined. Each annular reference region is characterized by an inner radius r_{in} and an outer radius r_{out} . The minimum inner radius, $r_{\text{in,min}}$, is estimated from a smoothing-spline approximation $s(x)$ of the central horizontal profile passing through $(x_{\text{c,step 1}}, y_{\text{c,step 1}})$. The transition between the spherical cap and the reference plateau is identified by the maxima of the absolute curvature $|\kappa(x)|$ of the spline located on either side of the centre position.

$$\kappa(x) = \frac{d^2}{dx^2}s(x) \left(1 + \left(\frac{d}{dx}s(x) \right)^2 \right)^{-\frac{3}{2}} \quad (2)$$

The two transition positions are

$$x_{\text{le}} = \underset{x < x_{\text{c,step 1}}}{\operatorname{argmax}} \{ |\kappa(x)| \}, \quad x_{\text{ri}} = \underset{x > x_{\text{c,step 1}}}{\operatorname{argmax}} \{ |\kappa(x)| \}. \quad (3)$$

The average distance of these transition points from the centre, i.e. half the distance between them, is used to define the radius of the inner bound $r_{\text{in,min,step 1}}$ of the reference plane.

$$r_{\text{in,min,step 1}} = \frac{1}{2}(x_{\text{ri}} - x_{\text{le}}) \quad (4)$$

The idea is, that the local curvature $|\kappa(x)|$ has its maximum value close to the transition of the spherical cap into the surrounding reference plateau. Therefore, $r_{\text{in,min,step 1}}$ represents an estimate of the radius of the smallest circle, which touches the border of the plane reference plateau outside of the cap.

The set of indices I_{cap} used for the subsequent fit of the spherical cap is defined by all data points located within a circular region centred at $(x_{\text{c,step 1}}, y_{\text{c,step 1}})$ with radius $r_{\text{in,min,step 1}}/3$:

$$I_{\text{cap}} = \left\{ (i, j) \mid (x_{i,j} - x_{\text{c,step 1}})^2 + (y_{i,j} - y_{\text{c,step 1}})^2 < \left(\frac{r_{\text{in,min,step 1}}}{3} \right)^2 \right\}. \quad (5)$$

A paraboloid is then fitted to the data points with indices $(i, j) \in I_{\text{cap}}$ to refine the estimate of the cap centre, yielding the updated coordinates $(x_{\text{c,step 2}}, y_{\text{c,step 2}})$.

Subsequently, a profile passing through the updated centre position is evaluated to refine the estimate of the minimum inner radius, resulting in $r_{\text{in,min,step 2}}$. The minimum inner radius $r_{\text{in,min,step 2}}$ around the center of the sphere cap at $(x_{\text{c,step 2}}, y_{\text{c,step 2}})$ contains all points, which are definitely not part of the surrounding reference plateau.

In case of `ana_DS_calib.py`, which uses a predefined width of the annulus as reference plane region and the minimum distance of the circumference to the center, an estimation of an inner radius of the reference annulus is not required. Here, step 2 directly uses this respectively the first center estimate.

To determine the outer radius, the Cartesian topography data are resampled into polar coordinates, that are uniformly distributed with respect to polar angles φ and that use $(x_{\text{c,step 2}}, y_{\text{c,step 2}})$ as the origin. For each angular coordinate φ , the maximum valid radial coordinate is determined and stored as $r(\varphi)$, thereby defining the outer boundary of the measurement object. The radii are determined for $n_\varphi = 360$ angle classes:

$$[\varphi_k, \varphi_k + \Delta\varphi), \quad \varphi_k = k\Delta\varphi \quad (6)$$

where

$$\Delta\varphi = \frac{\max\{\varphi_{(i,j)}\} - \min\{\varphi_{(i,j)}\}}{n_\varphi}, \quad \varphi_{(i,j)} = \arctan\left(\frac{y_{(i,j)}}{x_{(i,j)}}\right), \quad (i, j) \in V \quad (7)$$

and where V denotes the index set of data points lying inside the valid circular object area.

This is called by `analyse_depth` of `ana_DS_calib.py` where the variable `ref_width_micron` represents the user defined width of the annulus.

```

1 # Processing step 2:
2 #
3 radius_out_um = radius_circumference(
4     x_gridum, y_gridum, z_map_um,
5     psphere_um
6 )
7 radius_in_um = radius_out_um - ref_width_micron

```

The function `radius_circumference` is located in both main python programs calling `determine_DScircumference` from `algos_DSana`.

In case of `ana_DS_study.py` the set of admissible outer radii is defined as

$$r_{\text{out}} \in [\min\{r(\varphi)\}, \max\{r(\varphi)\}] \quad (8)$$

where r_{out} refers to a sample of radius values that are uniformly distributed along the radial coordinate with

$$\Delta r = \frac{\max\{r(\varphi)\} - \min\{r(\varphi)\}}{n_r}, \quad r_{\text{out},i} = \min\{r(\varphi)\} + i \Delta r \quad (9)$$

and where $i = 0, \dots, n_r$.

The admissible inner radii of the annular regions surrounding the cap are defined as

$$r_{\text{in}} \in [r_{\text{in,min,step 2}}, r_{\text{in,min,step 2}} + (\min\{r(\varphi)\} - r_{\text{in,min,step 2}})/2] \quad (10)$$

Fig. 2 illustrates the fitting regions used for the spherical cap and the reference plane. In general, the spherical cap is not perfectly centred with respect to the measurement object. Consequently, the reference-plane fitting region forms a complete annulus only for $r_{\text{out}} = \min\{r(\varphi)\}$.

Step 3: Definition and orientation of the annular reference plane

In the **third step**, the parameters of a regression plane

$$\hat{\mathbf{p}}_{\text{refplane}} = \underset{\mathbf{p}_{\text{pl}}}{\operatorname{argmin}} \left\{ \sum_{(i,j) \in I(r_{\text{in}}, r_{\text{out}})} (z_{i,j} - p_{0,\text{pl}}(x_{i,j} - x_{\text{c,step 2}}) - p_{1,\text{pl}}(y_{i,j} - y_{\text{c,step 2}}) - p_{2,\text{pl}})^2 \right\} \quad (11)$$

are fitted to the data points located within the annular region defined by the radii r_{in} and r_{out} with respect to the centre coordinates $(x_{\text{c,step 2}}, y_{\text{c,step 2}})$.

$$I(r_{\text{in}}, r_{\text{out}}) = \left\{ (i, j) \mid r_{\text{in}} < \sqrt{(x_{i,j} - x_{\text{c,step 2}})^2 + (y_{i,j} - y_{\text{c,step 2}})^2} < r_{\text{out}} \right\} \quad (12)$$

The complete data set is then translated and rotated such that the fitted reference plane coincides with the horizontal plane at $z_{\text{plane}} = 0$. The rotation aligns the surface normal with the optical axis using Rodrigues' rotation formula.

This is called by `analyse_depth` with

```

1 # plane fit and subsequent alignment
2 #
3 (
4     z_plateauplane_um ,
5     surface_normal , z_0 ,
6     cov_theta , sigma_resi
7 ) = algos_DSana.regression_plane(
8     x_gridum_shift , y_gridum_shift , z_map_um ,
9     idx_plateau
10 )
11
12 (
13     x_rot , y_rot , z_rot
14 ) = algos_DSana.rotate_by_surfacenormal(
15     x_gridum_shift , y_gridum_shift , z_map_um - z_0 ,
16     surface_normal
17 )
18
19 mean_z = np.mean(z_rot[idx_plateau])
20 z_rot -= mean_z

```

Step 4: Areal estimation of depth

In the **fourth step**, the depth of the spherical cap is estimated by fitting the parabolic model function given in Eq. (1) to the aligned data points with indices $(i, j) \in I_{\text{cap}}$, i.e. to the data points located inside the circular region defined in the second processing step.

$$\hat{\mathbf{p}}_{\text{cap}} = \underset{\mathbf{p}}{\operatorname{argmin}} \left\{ \sum_{(i,j) \in I_{\text{cap}}} (z_{i,j} - z_{\text{cap}}(\mathbf{p}, x_{i,j}, y_{i,j}))^2 \right\} \quad (13)$$

This is called by `analyse_depth` with

```

1 # fitting the parabola in step 4 according to center of
2 # parabola obtained in step 2
3 #
4 idx_sph = np.where(
5     (
6         ((x_gridum_shift)**2 + (y_gridum_shift)**2)
7         < (radius_in_um/3.)**2
8     )
9     & valid_fit
10 )
11 # -----
12 # fitting of the parabola to set of indices i_sph inside
13 # the circular disk identified during preprocessing
14 # now to the aligned data set
15 #
16 (
17     psphere_um_prime ,
18     sigma_pshp_um , covar_sph , sigma_resisph_um
19 ) = algos_DSana.fit_parabo(
20     x_rot[idx_sph].flatten() ,
21     y_rot[idx_sph].flatten() ,
22     z_rot[idx_sph].flatten() ,
23     drum ,
24     np.array([0. , 0. , psphere_um[2]])
25 )

```

Because the aligned reference plane is at $z = 0$, the areal depth is

$$d_A = -\hat{p}_{\text{cap},3}. \quad (14)$$

Equivalently, when the fitted plane level and cap-vertex level are expressed in the same un-aligned coordinate system,

$$d_A = \hat{p}_{\text{refplane},2} - \hat{p}_{\text{cap},3}. \quad (15)$$

In case of `ana_DS_study.py`, steps three and four are repeated for each reference region specified by a pair of radii $(r_{\text{in}}, r_{\text{out}})$.

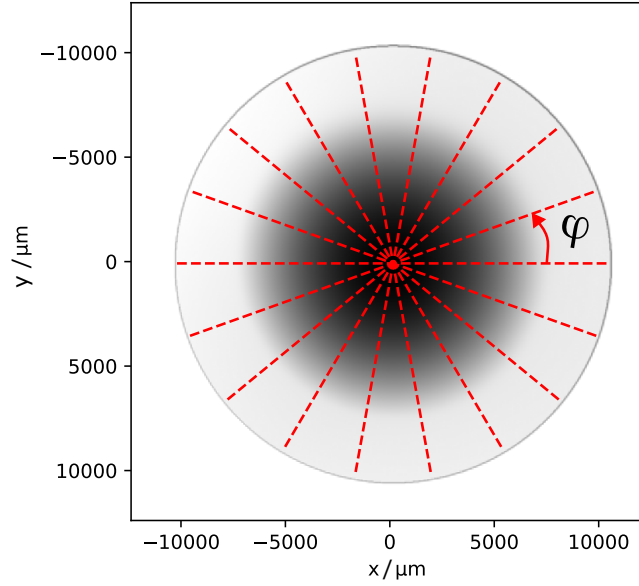


Figure 3: A finite set of radial profiles through the centre of the spherical cap is selected for a profilometric depth determination following the profile-based convention of ISO 5436-1.

3 Profile-based method:

In case of `ana_DS_study.py`, profile-based approaches are investigated. Instead of evaluating parallel profile traces, as is common for groove-shaped material standards, the profile-based analysis uses a finite number n_{prf} of radial cross-sectional profiles passing through the centre of the spherical cap, as illustrated in Fig. 3. Each profile is extracted from the aligned Cartesian data by quadratic interpolation, with the radial origin located at $(x_{\text{c,step 2}}, y_{\text{c,step 2}})$.

Each radial profile represents a diameter of the largest complete circular region, i.e. the region bounded by $\min\{r_{\text{out}}\}$. Since a profile at angle φ and a profile at angle $\varphi + 180^\circ$ describe the same diameter, the profile orientations are chosen in the interval $[0^\circ, 180^\circ)$. For n_{prf} equally spaced profiles, the angular increment is

$$\Delta\varphi_{\text{prf}} = \frac{180^\circ}{n_{\text{prf}}}. \quad (16)$$

The profile-based analysis is performed on the aligned data set, i.e. after rotation and vertical shifting according to the reference plane fitted to the annular reference region. Two variants of the profilometric evaluation are considered. In the first variant, the depth values are evaluated with respect to the common reference plane fitted to the annular region bounded by $r_{\text{in,min,step 2}}$ and $\min\{r(\varphi)\}$. In the second variant, each radial profile is referenced individually by fitting

a straight line to the profile points located within this annular region. For both variants, a parabola is then fitted separately to each radial profile, using only the profile points within the central interval

$$C = \left[-\frac{r_{\text{in,min,step 1}}}{3}, \frac{r_{\text{in,min,step 1}}}{3} \right]. \quad (17)$$

This is called by `analyse_depth` of `ana_DS_study.py` for one choice of annulus region with

```

1 # Profilometric processing for comparison:
2 #
3 if (i_ou==0) and (i_in==0):
4     n_samples = int(np.floor((r_limit_outer[0] - 10*dx_um) / dx_um))
5     (
6         angle_degree ,
7         depth_angular_cuts ,
8         zpos_on_forms
9     ) = analyse_Xsectprfs(
10         x_rot-psphere_um_prime[0] ,
11         y_rot-psphere_um_prime[1] ,
12         z_rot ,
13         r_inner_edge , r_limit_inner[-1] ,
14         n_samples , n_xsects ,
15         pltname
16     )
17     u_depth_prf = np.sqrt(cov_theta[2][2] + zpos_on_forms[2]**2)

```

Alignment with respect to overall reference plane:

For each radial profile, a regression parabola (rp) is fitted to the data points that lie inside the interval C with a width equal to one third of the cap diameter.

$$\hat{\mathbf{p}}_{\text{rp}}(\varphi) = \underset{\mathbf{p}}{\operatorname{argmin}} \left\{ \sum_{r_\nu \in C} (z_\nu(\varphi) - p_0 r_\nu(\varphi)^2 - p_1 r_\nu(\varphi) - p_2)^2 \right\} \quad (18)$$

As the entire data set has already been aligned to the reference plane by rotation and translation, the negative height of the fitted parabola minimum gives the depth $d_{\text{refplane}}(\varphi)$.

$$d_{\text{refplane}}(\varphi) = \frac{\hat{p}_{\text{rp},1}^2}{4\hat{p}_{\text{rp},0}} - \hat{p}_{\text{rp},2} \quad (19)$$

where $\hat{p}_{rp,0}$, $\hat{p}_{rp,1}$, and $\hat{p}_{rp,2}$ are the fitted quadratic, linear, and constant coefficients, respectively.

Alignment with respect to profiles:

For comparison with conventional procedures in which each profile has its own reference line, a straight line is fitted to the plateau portions of each radial profile. Let $z_{cp,refline}(\varphi)$ denote the height of this line at the lateral position r_{cp} of the fitted parabola minimum. The corresponding depth is

$$d_{refline}(\varphi) = d_{refplane}(\varphi) + z_{cp,refline}(\varphi), \quad (20)$$

where

$$z_{cp,refline} = \hat{p}_{rl,0} r_{cp} + \hat{p}_{rl,1} \quad (21)$$

and

$$r_{cp} = -\frac{\hat{p}_{rp,1}}{2\hat{p}_{rp,0}} \quad (22)$$

for each profile at directional angle φ .

4 Fit-derived uncertainties of height levels and depth estimates

All model parameters are estimated by least squares. Under the working assumption that the vertical residuals have zero mean, are mutually independent, are approximately normally distributed, and have a common variance, the least-squares parameter estimates coincide with the maximum-likelihood estimates. For a model $f(\mathbf{p}, \mathbf{q}_k)$ with observations z_k and lateral coordinates $\mathbf{q}_k$, the residuals are

$$\varepsilon_k(\mathbf{p}) = z_k - f(\mathbf{p}, \mathbf{q}_k), \quad k = 1, \dots, N. \quad (23)$$

For the areal method, the running index k enumerates the selected data points of the two-dimensional grid. Each value of k therefore corresponds to a pair of grid indices (i_k, j_k) , so that $\mathbf{q}_k = (x_{i_k, j_k}, y_{i_k, j_k})^\top$ and $z_k = z_{i_k, j_k}$. For the profile method, the data are one-dimensional and k directly enumerates the profile points, with $\mathbf{q}_k = r_k$.

The uncertainties of the fitted height levels and the resulting depth estimates are derived from the covariance matrices obtained from the least-squares fits. These matrices contain not only the variances of the fitted parameters but also their mutual covariances. The covariance terms must be retained when propagating the fit uncertainties to the evaluated height levels and

depths because the fitted parameters are generally correlated. Neglecting them may lead to either an overestimate or an underestimate of the uncertainty of the final depth value.

The usual first-order estimate of the parameter covariance matrix is

$$\mathbf{C}_{\mathbf{p}} \equiv \text{Cov}(\hat{\mathbf{p}}) \approx \hat{\sigma}_{\varepsilon}^2 (\mathbf{J}^{\top} \mathbf{J})^{-1}, \quad \hat{\sigma}_{\varepsilon}^2 = \frac{1}{N - M} \sum_{k=1}^N \varepsilon_k(\hat{\mathbf{p}})^2, \quad (24)$$

where M is the number of fitted parameters and

$$J_{k\ell} = \left. \frac{\partial \varepsilon_k}{\partial p_{\ell}} \right|_{\hat{\mathbf{p}}}, \quad \ell = 0, \dots, M - 1. \quad (25)$$

For the quadratic and straight-line profile models, the sign of the residual Jacobian $\mathbf{J}$ does not affect its product $\mathbf{J}^{\top} \mathbf{J}$. The corresponding design matrices are

$$\mathbf{R}_{\text{rp}} = \begin{pmatrix} r_{\text{rp},1}^2 & r_{\text{rp},1} & 1 \\ \vdots & \vdots & \vdots \\ r_{\text{rp},N_{\text{rp}}}^2 & r_{\text{rp},N_{\text{rp}}} & 1 \end{pmatrix}, \quad \mathbf{R}_{\text{rl}} = \begin{pmatrix} r_{\text{rl},1} & 1 \\ \vdots & \vdots \\ r_{\text{rl},N_{\text{rl}}} & 1 \end{pmatrix}, \quad (26)$$

where N_{rp} and N_{rl} are the numbers of points used for the regression-parabola and reference-line fits, respectively. Their covariance matrices are

$$\mathbf{C}_s = \hat{\sigma}_{\varepsilon,s}^2 (\mathbf{R}_s^{\top} \mathbf{R}_s)^{-1}, \quad \hat{\sigma}_{\varepsilon,s}^2 = \frac{1}{N_s - M_s} \sum_{k=1}^{N_s} \varepsilon_{s,k}^2, \quad s \in \{\text{rp}, \text{rl}\}, \quad (27)$$

with $M_{\text{rp}} = 3$ and $M_{\text{rl}} = 2$.

For a scalar quantity $g(\mathbf{p})$ derived from M fitted parameters, the sensitivity vector is

$$\mathbf{c}_g = \begin{pmatrix} \left. \frac{\partial g}{\partial p_0} \right|_{\hat{\mathbf{p}}} \\ \vdots \\ \left. \frac{\partial g}{\partial p_{M-1}} \right|_{\hat{\mathbf{p}}} \end{pmatrix}. \quad (28)$$

First-order covariance propagation then gives

$$u^2(g) = \mathbf{c}_g^{\top} \mathbf{C}_{\mathbf{p}} \mathbf{c}_g \quad \text{or} \quad u^2(g) = \mathbf{c}_g^{\top} \mathbf{C}_s \mathbf{c}_g. \quad (29)$$

In the present analysis, the scalar quantity g is the evaluated depth obtained using one of the

three approaches defined in Eqs. (14), (19), (20).

Where a result depends on parameters obtained from two different fits, the covariance terms between the two fitted parameter sets are taken to be zero. This is justified here because the fits are applied to disjoint sets of measured points: the reference-plane fit uses points within the annular reference region, whereas the cap fit uses points within the central region of the spherical cap. Within each fit, however, the complete covariance matrix is retained, including all covariance terms between the fitted parameters.

For the areal depth in Eqs. (14) and (15), the fit-derived variance is

$$\begin{aligned} u_{\text{fit}}^2(d_A) &= \text{Var}(\hat{p}_{\text{refplane},2}) + \text{Var}(\hat{p}_{\text{cap},3}) \\ &= u_{\text{plane}}^2(z) + u_{\text{cap}}^2(z). \end{aligned} \quad (30)$$

Although Eq. (14) expresses the depth as $-\hat{p}_{\text{cap},3}$ after alignment, the fitted reference-plane level that defines $z = 0$ is itself uncertain. Its variance must therefore be included in Eq. (30).

The resulting value characterizes the uncertainty of the fitted height levels within the least-squares model. It does not include spatial correlation of the residuals, deviations of the reference plateau from a plane, uncertainty associated with selecting the evaluation regions, or instrument-related effects.

For each profile angle φ , the regression parabola is

$$z_{\text{rp}}(r, \varphi) = p_{\text{rp},0}r^2 + p_{\text{rp},1}r + p_{\text{rp},2}. \quad (31)$$

For compactness, the hats and the explicit dependence of the fitted profile parameters on φ are omitted in the following equations. The depth of the parabola minimum relative to the globally aligned reference plane is

$$d_{\text{refplane}}(\varphi) = \frac{p_{\text{rp},1}^2}{4p_{\text{rp},0}} - p_{\text{rp},2}. \quad (32)$$

Its sensitivity vector with respect to the parabola parameters is

$$\mathbf{c}_{d,\text{refplane},\text{rp}} = \begin{pmatrix} \frac{\partial d_{\text{refplane}}(\varphi)}{\partial p_{\text{rp},0}} \\ \frac{\partial d_{\text{refplane}}(\varphi)}{\partial p_{\text{rp},1}} \\ \frac{\partial d_{\text{refplane}}(\varphi)}{\partial p_{\text{rp},2}} \end{pmatrix} = \begin{pmatrix} -\frac{p_{\text{rp},1}^2}{4p_{\text{rp},0}^2} \\ \frac{p_{\text{rp},1}}{2p_{\text{rp},0}} \\ -1 \end{pmatrix}. \quad (33)$$

The corresponding fit-derived variance is

$$u_{\text{fit}}^2(d_{\text{refplane}}(\varphi)) = \mathbf{c}_{d,\text{refplane},\text{rp}}^\top \mathbf{C}_{\text{rp}}(\varphi) \mathbf{c}_{d,\text{refplane},\text{rp}} + u_{\text{plane}}^2(z). \quad (34)$$

The last term accounts for the uncertainty of the common reference-plane level used to align the data set.

The profile-specific reference-line depth is

$$d_{\text{refline}}(\varphi) = \frac{p_{\text{rp},1}^2}{4p_{\text{rp},0}} - p_{\text{rp},2} - p_{\text{rl},0} \frac{p_{\text{rp},1}}{2p_{\text{rp},0}} + p_{\text{rl},1}, \quad (35)$$

where $p_{\text{rl},0}$ and $p_{\text{rl},1}$ are the slope and intercept of the reference line, respectively.

The sensitivity vector of $d_{\text{refline}}(\varphi)$ with respect to the parabola parameters is

$$\mathbf{c}_{d,\text{rp}} = \begin{pmatrix} \frac{\partial d_{\text{refline}}(\varphi)}{\partial p_{\text{rp},0}} \\ \frac{\partial d_{\text{refline}}(\varphi)}{\partial p_{\text{rp},1}} \\ \frac{\partial d_{\text{refline}}(\varphi)}{\partial p_{\text{rp},2}} \end{pmatrix} = \begin{pmatrix} -\frac{p_{\text{rp},1}^2}{4p_{\text{rp},0}^2} + \frac{p_{\text{rl},0}p_{\text{rp},1}}{2p_{\text{rp},0}^2} \\ \frac{p_{\text{rp},1}}{2p_{\text{rp},0}} - \frac{p_{\text{rl},0}}{2p_{\text{rp},0}} \\ -1 \end{pmatrix}. \quad (36)$$

With respect to the reference-line parameters, the sensitivity vector is

$$\mathbf{c}_{d,\text{rl}} = \begin{pmatrix} \frac{\partial d_{\text{refline}}(\varphi)}{\partial p_{\text{rl},0}} \\ \frac{\partial d_{\text{refline}}(\varphi)}{\partial p_{\text{rl},1}} \end{pmatrix} = \begin{pmatrix} -\frac{p_{\text{rp},1}}{2p_{\text{rp},0}} \\ 1 \end{pmatrix}. \quad (37)$$

The fit-derived variance of the profile-specific reference-line depth is therefore

$$u_{\text{fit}}^2(d_{\text{refline}}(\varphi)) = \mathbf{c}_{d,\text{rp}}^\top \mathbf{C}_{\text{rp}}(\varphi) \mathbf{c}_{d,\text{rp}} + \mathbf{c}_{d,\text{rl}}^\top \mathbf{C}_{\text{rl}}(\varphi) \mathbf{c}_{d,\text{rl}}. \quad (38)$$

Where a result depends on parameters obtained from the parabola and reference-line fits, the covariance terms between the two fitted parameter sets are taken to be zero. The fits are applied to disjoint sets of profile points, with the parabola fitted to the groove region and the reference line fitted to the surrounding reference regions. Within each fit, the complete covariance matrix is retained, including all covariance terms between the fitted parameters.

No additional term for the common reference-plane level appears in Eq. (38), because a com-

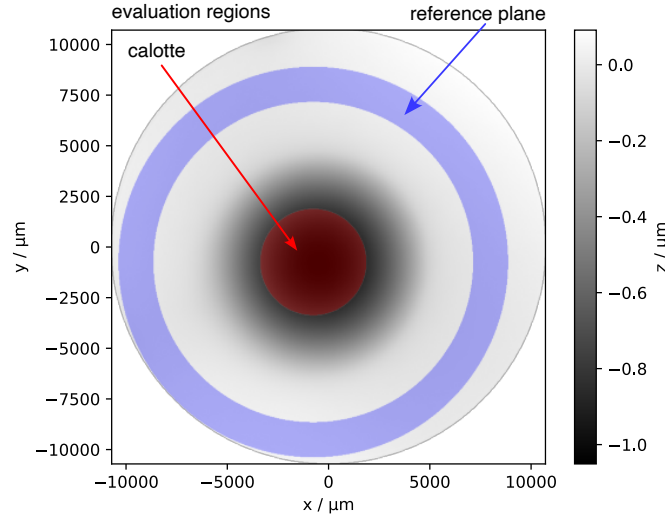


Figure 4: Height map of the $\alpha = 0^\circ$ orientation with evaluation regions indicated by highlighting, red for the spherical cap and blue for the annular ring of the reference surface.

mon vertical translation cancels in the difference between the reference-line and parabola levels.

For every pair $(r_{\text{in}}, r_{\text{out}})$, the areal depth d_A and its fit-derived standard uncertainty are calculated. The mean and standard deviation of the depths over all investigated reference regions are used separately to quantify the sensitivity to the definition of the reference region.

5 Standardized procedure for calibration services

A standardized procedure should maximize reproducibility between laboratories and instruments by fixing both the measurement configuration and the evaluation operator. The centre of the spherical cap should be positioned as close as practicable to the optical axis, and the annular reference region should be defined by a prescribed width measured inward from the largest complete circle contained within the valid object boundary.

The following evaluation steps are proposed:

1. determine the centre of the spherical cap, (x_c, y_c) ;
2. determine $r_{\text{ref,out}}$ as the minimum radial distance from the cap centre to the valid object boundary;
3. use the prescribed width w_{ref} of the annulus to determine the index set of the reference-

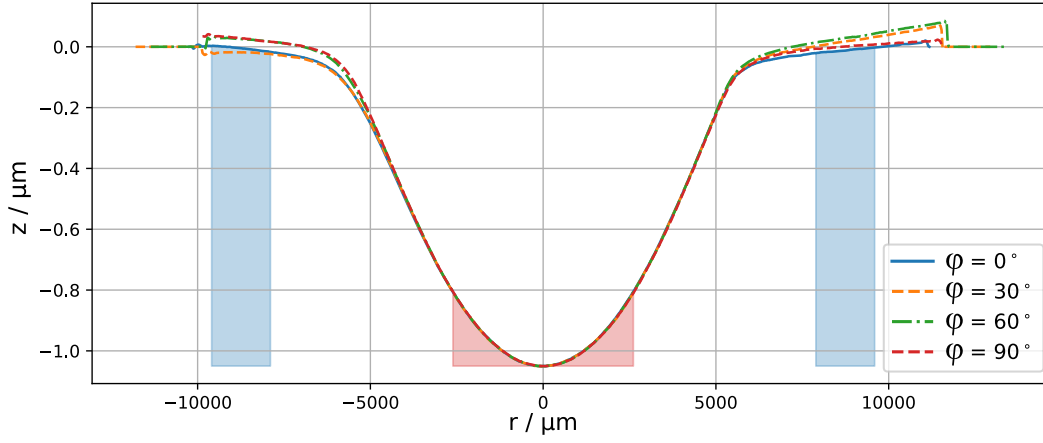


Figure 5: Four profiles of the $\alpha = 0^\circ$ object orientation at angular cross sections $\varphi = 0^\circ, 30^\circ, 60^\circ, 90^\circ$, with the evaluation regions indicated by highlighted areas under the curves: red for the spherical cap and blue for the annular region of the reference surface.

plane fit region, with inner radius $r_{\text{ref,in}} = r_{\text{ref,out}} - w_{\text{ref}}$ and outer radius $r_{\text{ref,out}}$;

4. translate the lateral origin to (x_c, y_c) and subtract the fitted plane height z_0 at that position;
5. rotate the complete data set so that the fitted plane normal is parallel to the vertical axis, and apply a final vertical shift so that the mean residual height in the reference annulus is zero;
6. fit the paraboloid in Eq. (1) to the central circular region of radius $r_{\text{ref,in}}/3$ and report the vertical separation between its vertex and the aligned reference plane as the depth d .

The spherical-cap centre is estimated in two steps. First, a circle is fitted to the locus of maximum slope. Subsequently, a paraboloid, Eq. (1), is fitted to the data lying inside that circle. The resulting centre (x_c, y_c) is used as the coordinate origin for the subsequent processing steps.

To characterize the repeatability of the measurements obtained with the same instrument and with a reference-annulus width of, for example, $w_{\text{ref}} = 1.75$ mm, the standard deviation of the mean, $u_{\text{rep}}(\bar{d})$, is calculated. The mean depth $\bar{d}$ and the corresponding standard deviation of the mean are given by

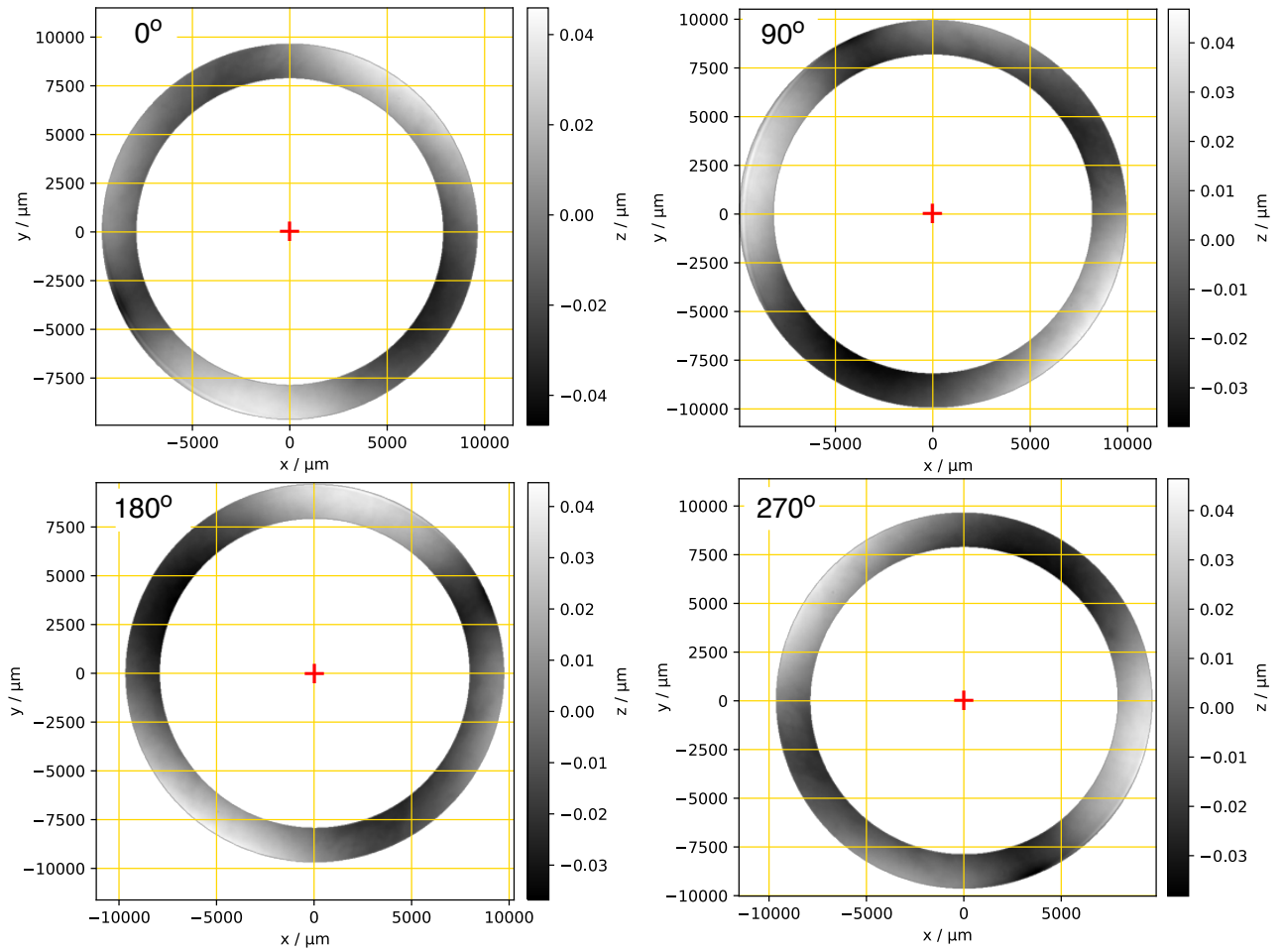


Figure 6: Reference-surface regions for the four orientations $\alpha = 0^\circ, 90^\circ, 180^\circ, 270^\circ$, showing the form deviation of the depth standard.

$$\bar{d} = \frac{1}{n_{\text{meas}}} \sum_{m=1}^{n_{\text{meas}}} d_m, \quad (39)$$

and

$$u_{\text{rep}}(\bar{d}) = \frac{\sigma_d}{\sqrt{n_{\text{meas}}}}, \quad \sigma_d = \sqrt{\frac{1}{n_{\text{meas}} - 1} \sum_{m=1}^{n_{\text{meas}}} (d_m - \bar{d})^2}. \quad (40)$$

where n_{meas} is the number of measurements and σ_d is the standard deviation of the individual depth values.

A CSV file is written with one row for each data set. It contains the filename, the evaluated depth, the fit-derived standard uncertainty, the standard deviations of the plane-fit and cap-fit

Table 1: Measurements at four different orientations α performed at PTB and one measurement result obtained from an independent laboratory.

α	$d/\mu\text{m}$	$u_{\text{fit}}(d)/\mu\text{m}$	$\sigma_{\text{resi,plane}}/\mu\text{m}$	$\sigma_{\text{resi,cap}}/\mu\text{m}$
0°	1.05000	0.00006	0.01984	0.00104
90°	1.05170	0.00006	0.01983	0.00105
180°	1.05067	0.00006	0.01947	0.00113
270°	1.05389	0.00006	0.02035	0.00118

residuals, and the measurement date and time. The fit-derived standard uncertainty $u_{\text{fit}}(d)$ is propagated from the covariance matrices of the fitted parameters according to Eq. (30).

The four representative data sets provided in the repository give the following results when evaluated with $w_{\text{ref}} = 1.75 \text{ mm}$ and with a lateral resolution (pixel size) of $29.30 \text{ }\mu\text{m}$.

The repository provides only a small number of data sets because they are intended as implementation examples. A characterization or calibration should be based on a larger number of measurements.

For the four example measurements shown in Table 1, the mean depth calculated according to Eq. (39) and the experimental standard deviation of the mean calculated according to Eq. (40) are

$$\boxed{\bar{d} = 1.05157 \mu\text{m}} \quad (41)$$

and

$$\boxed{u_{\text{rep}}(\bar{d}) = 0.85 \text{ nm.}} \quad (42)$$

Here, $u_{\text{rep}}(\bar{d})$ characterizes the repeatability represented by the four rotational orientations, with one measurement for each orientation only, rather than the repeatability of consecutive measurements at a fixed orientation.

Different instruments and laboratories may differ slightly in their lateral-scale calibration and in the detected object boundary. Both effects change the physical position and width of the annulus represented by a prescribed set of pixels. Their influence on the evaluated depth was estimated by repeating the evaluation using

$$w_{\pm} = w_{\text{ref}} \pm \Delta w, \quad \Delta w = 0.5 \text{ mm.} \quad (43)$$

For the example data, this gives $w_- = 1.25 \text{ mm}$ and $w_+ = 2.25 \text{ mm}$. If the unknown effective annulus width is assumed to be uniformly distributed over this interval, the associated standard uncertainty can be estimated from the full change in depth as

$$u_{\Delta w}(d) = \frac{|d(w_+) - d(w_-)|}{2\sqrt{3}}. \quad (44)$$

The depth values obtained for the limiting annulus widths are summarized in Table 2.

Using the largest observed full difference, 5.12 nm, gives

$$\boxed{u_{\Delta w}(d) = 1.48 \text{ nm.}} \quad (45)$$

This estimate is conditional on the assumed rectangular distribution. Where traceable infor-

Table 2: Variation of the depth values obtained for the four orientations α when the width of the reference annulus is varied.

α	$w_- = 1.25\text{mm}$	$w_+ = 2.25\text{mm}$	$ d(w_+) - d(w_-) $
0°	$1.05229\ \mu\text{m}$	$1.04751\ \mu\text{m}$	$0.00478\ \mu\text{m}$
90°	$1.05418\ \mu\text{m}$	$1.04906\ \mu\text{m}$	$0.00512\ \mu\text{m}$
180°	$1.05302\ \mu\text{m}$	$1.04813\ \mu\text{m}$	$0.00489\ \mu\text{m}$
270°	$1.05622\ \mu\text{m}$	$1.05136\ \mu\text{m}$	$0.00486\ \mu\text{m}$

mation on the lateral-scale calibration and a quantitative uncertainty associated with boundary detection are available, their effects should instead be propagated separately.

The influence of the lateral scale for these example data was additionally assessed by varying the assumed pixel size by 6.55 %. The resulting full difference between the evaluated depth values was $\Delta d = 0.54\ \text{nm}$. Approximating the distribution by a rectangular distribution gives

$$u_{\text{lat}}(d) = \frac{\Delta d}{2\sqrt{3}}, \quad \Delta d = 0.54\ \text{nm}. \quad (46)$$

The uncertainty of the pixel size is correlated with the change in physical position and width of the annulus represented by a prescribed set of pixels. A corresponding correlation term has not been estimated here. Previous investigations on the instrument with which the data in the repository were acquired yielded a value of $u_{\text{lat}} = 1\ \text{nm}$ for the contribution due to uncertainties of the lateral scaling. The larger value is therefore used below as a conservative upper limit.

The standard uncertainty $u_c(d)$ of the depth determination is obtained by combining the instrumental and environmental uncertainty contributions of the experimental setup with the uncertainty contributions associated with the evaluation of the depth standard. Its square is given by

$$\begin{aligned} u_c^2(d) = & u_{\text{flat}}^2(d) + u_{\Delta w}^2(d) + u_{\text{T}}^2 + u_{\text{lat}}^2(d) \\ & + u_{\text{rep}}^2(\bar{d}) + u_{\text{ret}}^2 + u_{\lambda}^2 + u_{\text{fit}}^2(d). \end{aligned} \quad (47)$$

The uncertainty contributions considered in this example are summarized in Table 3. Using a coverage factor of $k = 2$, the expanded uncertainty is $U = 9.77\ \text{nm}$. The measurement result for the example with one measurement at each of the four orientations of D23 is therefore

Table 3: Exemplary uncertainty budget for measurements at four different orientations α performed using PTB's flatness-measurement interferometer.

Contribution	Symbol	Value
reference flat	$u_{\text{flat}}(d)$	4.33 nm
reference-annulus width	$u_{\Delta w}^2(d)$	1.48 nm
temperature	u_{T}	1 nm
lateral scaling	u_{lat}	1 nm
repeatability	$u_{\text{rep}}(\bar{d})$	0.85 nm
retrace errors	u_{ret}	0.5 nm
plane and paraboloid fits	$u_{\text{fit}}(d)$	0.06 nm
light wavelength	u_{λ}	0.05 nm
combined standard uncertainty	$u_{\text{c}}(d)$	4.88 nm
expanded uncertainty for $k = 2$	$U(d)$	9.77 nm

$$d = (1.05157 \pm 0.00977) \mu\text{m} \quad (48)$$