Effects of rotation errors on goniometric measurements

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Goniometric measurements are essential for the determination of many optical quantities. Quantifying the effects of errors in the rotation axes on these quantities is a complex task. In this paper, we show how a measurement model for a four-axis goniometric system can be developed. We then investigate how the uncertainties due to several error sources propagate to the rotation angles and then through to the measurement of bi-directional reflectance.

GONIOMETRIC MEASUREMENTS

Many spectrophotometric and photometric quantities depend critically on the geometry of measurement. The bidirectional reflectance distribution function (BRDF) for materials, for example, is a function of the polar and azimuthal angles of incidence of light, θ_i and ϕ_i, as well as the polar and azimuthal angles of detection of reflected light, θ_d and ϕ_d. Instruments for measurement of BRDF, therefore, must contain four axes to span the parameter space.

Despite the best efforts of the instrument designers, each rotation using these axes will be subject to errors, including:

- displacement of the centres of rotation of the axes;
- misalignment (non-orthogonality) of the axes;
- angular resolution of the axis motors;
- angular accuracy of each axis;
- determining the zero angle of each axis.

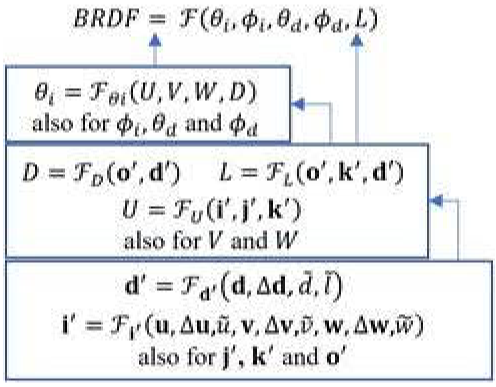
This work describes an approach for assessing the uncertainty of BRDF associated with these errors.

MEASUREMENT MODEL

To capture the effect of various errors on a measured quantity, a measurement model must be constructed. The measurement model expresses the measurand in terms of all input parameters, including the errors (even the errors have been corrected for, and the best estimate is zero, they will carry a standard uncertainty through the equations). The measurement equation should account for the components of the system that define the axes – for example in the MSL system, the *z*-axis is defined by the incident beam and, therefore, there is no uncertainty in the alignment of this beam, but rather in all other axes relative to it.

If the rotations are controlled in a coordinate system different to that of the measurand, the transformations between coordinate systems are part of the measurement model. For example, at MSL the angle of a detector, D, is set on a slew ring and the sample placed on orthogonal axes rotating about lab *x*-, *y*- and *z*-axes by angles U, V and W. However, BRDF is generally defined in θ_i, ϕ_i, θ_d, ϕ_d space.

The measurement equation(s) therefore consist, in MSL's case, of the following, considering only the parameters relating to the four rotation axes:



Here: L and $\tilde{l}$ are the true and measured distances from the sample to the detector; d is the measured value of D; $\mathbf{d}$ and $\Delta\mathbf{d}$ define the slope of the detector axis and its displacement from the origin; $\mathbf{i}'$, $\mathbf{j}'$, and $\mathbf{k}'$ are rotated basis vectors and $\mathbf{o}'$ is origin rotated by angles $\tilde{u}$, $\tilde{v}$ and $\tilde{w}$ about the axes defined by the vectors $\mathbf{u}$, $\mathbf{v}$ and $\mathbf{w}$ displaced by $\Delta\mathbf{u}$, $\Delta\mathbf{v}$ and $\Delta\mathbf{w}$ respectively. The axis vectors and displacements are given by (for example):

$$\Delta\mathbf{w} = \left[E_{\Delta W_x}, E_{\Delta W_y}, 0\right] \quad \mathbf{w} = \mathbf{k} - \left[E_{W_x}, E_{W_y}, 0\right],$$

where the $E_{\Delta W}$ are displacement errors and the E_W are misalignment errors. These errors are assumed to be distributed with zero mean. The angles of rotation about these axes are given (for example) by:

$$\tilde{w} = w - E_{W\_\mathrm{resolution}} - E_{W\_\mathrm{accuracy}} - E_{W\_\mathrm{zero}}.$$

Here, w is the measured angle to which the axis is set and the E_W are the last three errors identified in the bullet points in the previous section.

The uncertainties associated with the five errors identified have been included in the measurement model and can be propagated through the coordinate systems to the BRDF. The forms of the functions given above can be found in the literature (e.g., [1] for the transformation from $UVWD$ to $\theta_\text{i}\ \phi_\text{i}\ \theta_\text{d}\ \phi_\text{d}$). The position of a point **a** (expressed as a vector) after rotation about a displaced and misaligned axis is:

$$\mathbf{a}' = \mathbf{R}(\hat{\mathbf{w}}, \tilde{w})(\mathbf{a} - \Delta\mathbf{w}) + \Delta\mathbf{w},$$

where $\mathbf{R}(\hat{\mathbf{w}}, \tilde{w})$ is the rotation matrix for an angle $\tilde{w}$ about the vector $\hat{\mathbf{w}}$ (**w** normalised to unit length). To rotate the basis vectors, each end of the vector (the origin and the tip of the vector) should be rotated and their difference found. If the sample is on a three-axis stage, the rotation about the respective axes are carried out sequentially, and in an order that depends on the specifics of the system being used.

ERROR PROPAGATION

Three methods of error propagation through the measurement equations have been used and compared. Firstly, distributions have been assigned to each of the sources of error and Monte Carlo simulations have been carried out by drawing samples from those distributions and calculating the standard deviation of the results. Secondly, the sensitivity coefficients of the outputs on the error contributions (e.g., $\partial\theta_\text{i}/\partial E_{W_x}$) have been evaluated analytically and the GUM [2] methods used to propagate the uncertainties. Thirdly, the GTC [3] Python tool for the automatic propagation of uncertainty, has been used. It was found that all three methods produced the same propagated uncertainties. However, GTC was the most straightforward to use and delivers correlations between quantities (e.g., $u(\theta_\text{i}, \phi_\text{i})$) without any additional effort.

Figure 1 shows the standard uncertainty in θ_i, ϕ_i, θ_d and ϕ_d as a function of the v angle when u is 30°, w is 0° and d is 30°. The standard uncertainty associated with each displacement is 0.02 % of the radius of the system, with each misalignment is 0.06° and with each accuracy is 0.05°. The resolution and zero position errors are negligible.

BRDF AND TOTAL REFLECTANCE

Of more interest is the contribution of rotation errors on the final measurand: the BRDF or the integrated BRDF if, for example, total hemispherical reflectance is required. As a simple example, the uncertainty in BRDF of a Lambertian material measured in 0°:x° and in x°,180°:45°,0° geometries is shown in Fig. 2.

In the 0°:x° data we can see that propagated uncertainties increase with the sensitivity to θ_d (the uncertainty of which is found to be primarily due to the accuracy errors in the **v** and **d** axes). In the

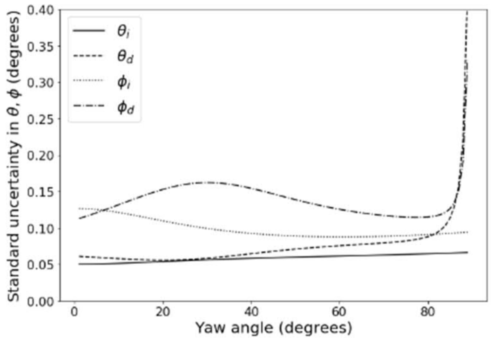


Figure 1. Standard uncertainties of θ_i, ϕ_i, θ_d and ϕ_d as a function of the v angle when the rotation uncertainties are as given in the text.

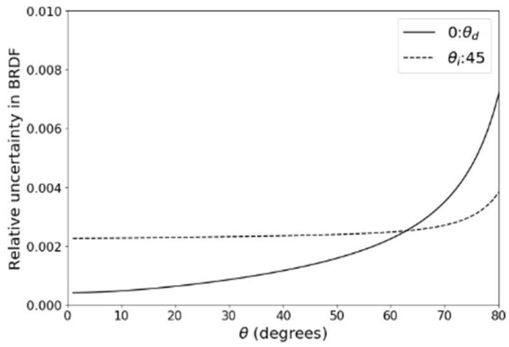


Figure 2. Standard uncertainties in the BRDF of Lambertian material measured in 0°:x° and in x°,180°:45°,0° geometries.

x°,180°:45°,0° data, on the other hand, where θ_d is fixed, the uncertainty is constant across most of the range and is dominated by the uncertainty in L induced by the misalignment of the **w** axis under a 180° rotation.

If integrating, then covariances between the BRDF measured at one angle and that measured at another angle must be known for a robust estimate of the uncertainty. In this case, the intrinsic nature of the GTC package becomes invaluable as these are taken account of with no extra effort by the analyst. For example, when calculating the total reflectance of a Lambertian sample, the uncertainty is 0.06 %, dominated again by the uncertainty in L but this time induced by the uncertainty in displacement of the **d** axis.

REFERENCES

1. T. Germer and C. Asmail, Goniometric optical scatter instrument for out-ot-plane ellipsometry measurements, Rev. Sci. Instrum., 70, 3688, 1999.
2. JCGM, JCGM 100:2008, Evaluation of measurement data – Guide to the expression of uncertainty in measurement, BIPM, 2008.
3. B. D. Hall, Object-oriented software for evaluating measurement uncertainty, Measurement Science and Technology, 24, 055004, 2013.