Study of Uncertainty Sources in Incident Angle Dependence of Regular Reflectance and Transmittance using a STAR GEM Accessory

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Abstract. *The study of uncertainty sources is carried out to evaluate the performance of a new developed instrument. The sources of the uncertainties are listed according to the uncertainties induced not only by optical scatterings, non-linearity of a detector and imperfections and surface roughness of used ellipsoidal mirrors but also by misalignments concerning many degrees of freedom of translation and rotation of the instrument. Many uncertainties will be estimated by Type A method.*

Keywords: Uncertainty Estimation, STAR GEM, Absolute Reflection, Symmetry X System

1. Introduction

Though a huge number of optical accessories to measure reflectance (*R*) and/or transmittance (*T*) have been proposed and several have been realized [1], an accessory, which is devised to measure both *R* and *T* with the same accuracy, was close to nil [2],[3]. Such an accessory is an important but really difficult product, because the absorptance of non-absorbing samples, which can be obtained from the measured *R* and *T* of specular samples according to energy conservation, should be zero. Furthermore, an accessory, which can measure the incident angle dependence of the absolute *R,* was only a gonio-reflectometer. A new developed STAR GEM accessory can absolutely measure both regular *R* and regular *T* with the same accuracy at an incident angle from 0 to 90 degrees. This paper is a scheme drawing of the uncertainty estimation of *R* measured by the STAR GEM.

2. Description of the STAR GEM

The STAR GEM, which consists of two equivalent belt-shape ellipsoid mirrors of revolution (E1 and E2) in Fig.1, 2 and 3, can continuously change both an angle of incidence and that of collection independently. The STAR GEM, which is constructed on the basis of the Symmetry X idea [3], can absolutely measure both regular *R* and *T* with the same accuracy. These measured *R* and *T* are independent each other, because a rotation angle (ψ) of the RM2 mirror in Fig.2 is automatically fine-turned in order to always search the rotation angel (ψ_0), which gives us the maximum intensity of each signal in every six modes [4].

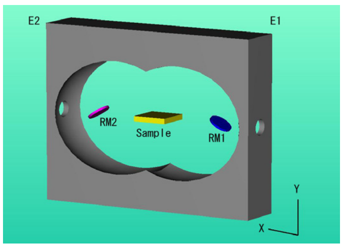

Fig.1. 3D figure of the GEM

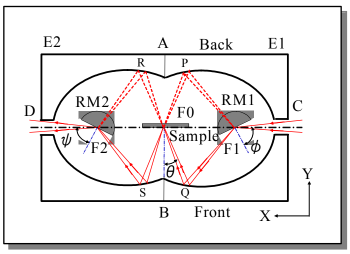

Fig.2. Cross section along meridian plane

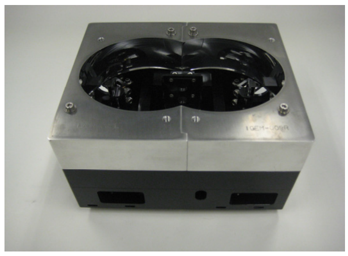

Fig.3. STAR GEM Type1

3. Measurement system

An optical setup to estimate the uncertainty is shown in Fig.4. An illuminator consists of a halogen lamp (HL), a band pass filter (F1), a neutral density filters (F2), a light chopper (LC), a beam-splitter (WW1), a monitor receiver, a space filter (SF), a parabolic mirror (PM1), a beam-splitter (WW2) and a polarizer (PO). The radiant flux through the polarizer enters the STAR GEM Type1 and is focused

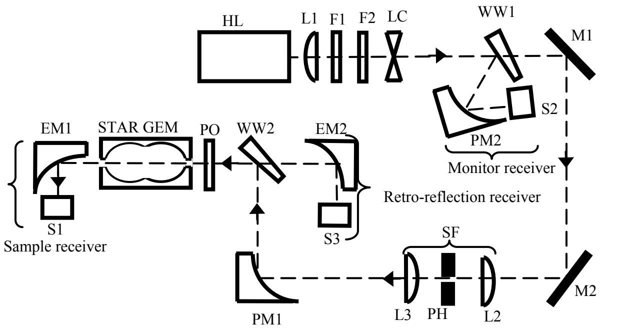

Fig.4. Schematic to measure uncertainty of STAR GEM

on the F1 focus in Fig.2 by the PM1 mirror. After an interaction with the sample or a non-interaction for a background measurement, the exiting flux is measured by a sample receiver. The receiver consists of an ellipsoidal mirror (EM1), a silicon photodiode detector (S1) and a lock-in amplifier. For this study, the RM1 and RM2 mirrors and the STAR GEM itself are held on multi-axes linear and rotational stages. A line connecting between the halogen lamp and the detector is called an external axis. The direction of light propagation is an X-axis and that of sample translation is a Z- axis. A sample was a non-absorbing and parallel-plate fused quartz and its shape was a disk of a 40-mm diameter and 1-mm thickness with specular surfaces.

4. Measurement Equation and Uncertainty Analysis

Although the STAR GEM can measure both R and T, at first we estimate the uncertainty of the reflectance measured by the STAR GEM. This paper treats the case where all variables, Q_1, Q_2, …., Q_N, are independent. A measured R is determined from these variables through a functional relationship f:

$$R = f(Q_1, Q_2, ..., Q_N) \tag{1}$$

The standard uncertainty of r, where r is the estimate of the measured R and thus the result of the measurement, is obtained by combining the standard uncertainties of the variable estimates q_1, q_2,.., q_N. The combined standard uncertainty $u_c(r)$ is the positive square root of the combined variance $u_c^2(r)$,

$$u_c^2(r) = \sum_{i=1}^{N} \left(\frac{\partial f}{\partial q_i} \right)^2 u^2(q_i) \tag{2}$$

where each $u(q_i)$ is a standard uncertainty evaluated in Type A evaluation or in Type B evaluation. The partial derivatives $\partial f / \partial q_i$ are called sensitivity coefficients and are sometimes determined experimentally: one measures the change in R produced by a change in a particular Q_i while holding the remaining variable quantities constant.

5. Sources of uncertainty

One ellipsoidal mirror possesses two foci. This natural feature was considered as a merit for a reflectometer, where a sample and a detector were put on each focus. Until the middle of 1980's, many scientists studied about the reflectometer using a hemi-ellipsoidal mirror. However, all investigations failed and there is no reflectometer using the ellipsoidal mirror today. Dr. K.A. Snail and Dr. L.M. Hansen [1] enumerated eight problems. They are the misalignment of the sample and detector, the inter-reflection between two foci and ellipsoidal mirror imperfections and so on. The sources of the uncertainty exist in the STAR GEM, in the illuminator, in the sample, in the receiver and so on. In the following, each source of uncertainty is chosen to be independent each other and is considered separately.

(A) STAR GEM Type1

(1) Misalignment between the GEM axis and the external axis

Three degrees (X, Y, and Z) of freedom of translation and two degrees (Y-axis and Z-axis) of freedom of rotation induce the uncertainty concerning a misalignment between two axes. The translation along X-axis makes the beam spot on the RM1 mirror blur, because the distance between PM1 and RM1 changes. The translations along Y-axis and Z-axis increase the distance between two axes. The rotations around Y-axis and Z-axis at the center of the F1 focus degenerate the degree of parallelization between two axes. In order independently to estimate the uncertainties of 5 categories, the change in R produced by a change in a particular freedom is measured, while holding the remaining degrees of freedom constant. A remaining degree (X-axis) doesn't induce the uncertainty, because the beam entering into the STAR GEM has the symmetry of rotation around the external axis.

(2) Misalignment between the F1 focus and the RM1 mirror
Two degrees (X and Y) of freedom of translation induce the uncertainty concerning a misalignment between the F1 focus and the RM1 mirror. A degree (Z-axis) of freedom of rotation induces the uncertainty of the incident angle. A remaining degree (Z) of freedom of translation doesn't induce the misalignment because of translation on the RM1 mirror. Another degree (X-axis) of freedom of rotation makes the RM1 mirror tilt to the meridian plane in Fig.2. But this doesn't induce the uncertainty because of the revolving ellipsoidal mirrors. This is an advantage of the STAR GEM but the gonio-reflectometer doesn't possess this. The other (Y-axis) makes the RM1 mirror rotate around its normal, so that this doesn't induce the uncertainty.

(3) Misalignment between the F2 focus and the RM2 mirror
Two degrees (X and Y) of freedom of translation induce the uncertainty concerning a misalignment between the F2 focus and the RM2 mirror. The degree (Z-axis) of freedom of rotation is the rotation of the RM2 mirror and its uncertainty is considered to be zero, because the RM2 is automatically fine-turned in order to always search the rotation angel, which gives the maximum intensity. The remaining three degrees are the same reasons in Sec.(2).

(4) Misalignment between the F0 focus and the sample
Two degrees (X and Y) of freedom of translation induce the uncertainty concerning a misalignment between the F0 focus and the sample. Two degrees (X-axis and Z-axis) of freedom of rotation tilt to the meridian plane and rotate the sample, respectively. The tilt induces the uncertainty concerning a misalignment because of the fall of the Symmetry X system. The rotation induces the uncertainty of not only incident angle but also the position of beam on the E2 mirror especially for the reflection measurement. Two remaining degrees of freedom of Z-translation and Y-axis-rotation don't induce the misalignment but move the beam on the sample surface. These are estimated in Sec. (8).

(5) Inter-scattering in the STAR GEM induced by a transparent sample
When either reflection or transmission measurement of a transparent sample is made, either transmission light or reflection light remains inside the STAR GEM and emerges stray-light due to scattering from the rear of the RM2 mirror, respectively. The intensity is measured by the retro-reflection receiver.

(B) Illuminator

(6) Stray-light of light source
The stray-light is radiant flux that reaches the detector at wavelengths outside the nominal spectral bandwidth of the band pass filter. The intensity of the stray-light is different whether the reflection, the transmission or the background measurements is made, because reflectance and transmittance of the sample aren't equal to unity. The uncertainty is estimated by Type B evaluation.

(7) Uncertainties in wavelength setting and in polarizer setting
The uncertainties are induced due to error of the center wavelength of the band pass filter and due to error of the rotation angle of the polarizer.

(C) Sample

(8) Non-uniformity of the sample
When the non-absorbing and parallel-plate sample is illuminated by incoherent light, there is no parameter concerning the sample thickness, which directly affects the sample signals. The uncertainty, which is induced by the non-uniformity of the sample, is counted by increase of signal noise mentioned in Sec. (13).

(9) Scattering and diffraction from the sample
The scattering and diffraction from the sample induce the uncertainty of sample signals. The intensity is measured by the measurement of the maximum profile.

(D) Receiver

(10) Nonlinearity of the detector
The nonlinearity of the Si-photodiode detector is a possible source of uncertainty. The nonlinearity results in the ratio of the signals not being equal to the ratio of the reaching fluxes. Nonlinearity also may arise within the ranges of the lock-in amplifier.

(11) Non-uniformity of the detector

While the RM2 mirror of the STAR GEM in Fig.2 is rotated little by little angle to find the maximum intensity of each signal in every six modes, the flux exiting from the STAR GEM is focused on the detector by the EM1 mirror in Fig.4 and is moving on the sensitive area of the detector. The non-uniformity of the detector induces the uncertainty.

(12) Retro-reflection from the detector

There is no inter-reflection between two foci of the STAR GEM different from a previous reflectometer using a hemi-ellipsoidal mirror. The reflection from a window of the detector in Fig.4 may cause the retro-reflection through the STAR GEM. The intensity is measured by the retro-reflection receiver.

(E) Others

(13) Signal noise

A signal noise is the result of random processes in both the sample and monitor receivers, in the optical source, in the sample and in the STAR GEM such as imperfections and surface roughness of the GEM.

Table 1 Uncertainty estimations

	Class	Variables	Measurements
A	STAR GEM	14+1	14 degrees of translation and rotation and scattering from the rear of RM2
B	Illuminator	2+1	Two errors and stray-light from the band-pass filter
C	Sample	1	Scattering from the sample
D	Detector	2+1	Two error and scattering from the window of the detector
E	Others	1	Signal noise
Total		$N = 23$	

6. Discussion

There are few papers about uncertainty estimations of optical accessories, except a gonio-reflectometer [5]. Because of the simple structure of the gonio-reflectometer, its estimation of the standard uncertainty of measurement isn't complex. However, it was difficult to construct the STAR GEM, which can measure *R* and *T* spectra with high accuracy. The main sources of the uncertainty are considered to be the optical alignment from our experience. 23 categories for the uncertainty estimations in Table 1 are too many, but 60 % is concerning to the alignments. It is considered that the detailed analysis of uncertainties may make the suggestion of a new construction way and a new alignment method. Next we evaluate the uncertainty of *T* measured by the STAR GEM at the same time and also evaluate the covariance between *R* and *T*. This makes the degree of independence between *R* and *T* clear from the view of the Statistics.

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