Interpolation of Spectral Responsivity of Trap Detectors and Evaluation of Measurement Uncertainties Using Monte Carlo Method

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This paper describes how the Standards and Calibration Laboratory interpolates the responsivity of trap detectors measured by a cryogenic radiometer at 7 wavelengths to the spectral range 400 nm to 800 nm and evaluates the uncertainties using Monte Carlo method.

INTRODUCTION

The Standards and Calibration Laboratory (SCL) has recently set up a cryogenic radiometer for calibration of spectral responsivity of trap detectors built from silicon photodiodes. The spectral responsivity, denoted by $S_{i,\ i\ =\ 1\ to\ 7}$, are measured at the output wavelengths of a krypton ion laser, namely 406.7 nm, 413.1 nm, 476.2 nm, 530.9 nm, 568.2 nm, 647.1 nm and 799.3 nm. To apply the trap detector for measurement work, these results need to be interpolated to the spectral range of 400 nm to 800 nm and the measurement uncertainties evaluated. The interpolation can be performed by purely mathematical functions such as polynomials or by fitting a physical model for the photodiodes [1]. SCL adopts the latter way to perform the interpolation. This paper also describes how the uncertainties are evaluated using Monte Carlo method (MCM).

RESPONSIVITY MODEL

The spectral responsivity $S(\lambda)$ at wavelength λ is given by,

$$S(\lambda) = \frac{(1-r(\lambda))\eta_i(\lambda)n_{air}\lambda e}{hc} \tag{1}$$

where $r(\lambda)$ and $\eta_i(\lambda)$ are the reflectivity and internal quantum efficiency of the photodiode, n_{air} is the refractive index of air, e is the electron charge and h is the Planck constant. $\eta_i(\lambda)$ can be obtained using the following equation [2][3],

$$n_i(\lambda) = P_f + \frac{1-P_f}{\alpha(\lambda)T}\left(1-e^{-\alpha(\lambda)T}\right) - \frac{1-P_b}{\alpha(\lambda)(D-T)}\left(e^{-\alpha(\lambda)T} - e^{-\alpha(\lambda)D}\right) - P_b e^{-\alpha(\lambda)w} + R_{back}e^{-\alpha(\lambda)w}P_b \tag{2}$$

where $\alpha(\lambda)$ and w are the absorption coefficient and thickness of the photodiode, P_f is the collection efficiency at the silicon dioxide/silicon interface and P_b is the value at the bulk, T is the depth of the p-n junction and D is the depth of the bulk region. R_{back} is the reflection coefficient at the back of the photodiode and this term is only required for interpolation to wavelengths longer than 920 nm [2]. Its value is treated as zero in this paper.

An interpolation function for $\alpha(\lambda)$ is given in [3] as follows where A_1 = 0.53086 μm^{-1}, A_2 = 0.469643 μm, A_3 = -0.28801 μm^{-2} , A_4 = -0.988739, A_5 = 0.282028 μm^{-1} and λ_0 = 0.256897 μm.

$$\alpha(\lambda) = A_1 e^{\frac{A_2}{(\lambda-\lambda_0)}} + A_3\lambda + A_4\lambda^{-1} + A_5 \tag{3}$$

The reflectivity $r(\lambda)$ takes the following form with the parameters obtained from prior information or by fitting [3]. In this paper the parameters for $r(\lambda)$ are not fitted since there are insufficient data.

$$r(\lambda) = ae^{\frac{b}{\lambda}} + c\lambda + d \tag{4}$$

INTERPOLATION PROCEDURE AND UNCERTAINTIES EVALUATION

The responsivity $S(\lambda)$ is calculated using (1) to (4). The 4 parameters (P_f, T, P_b, D) of the model are obtained by least squares fitting to the S_i data. The thickness w is assigned a value of 400 μm and not fitted. The Nelder-Mead (NM) algorithm [4] is used for searching the minimum of the residual error.

The interpolation procedure can be viewed as a measurement model in the GUM framework (GUF) [5] having S_i as input quantities and the responsivity $S(\lambda)$ as output quantity. Since the NM algorithm is not a differentiable function, the GUF might not be directly applicable to derive the uncertainties of $S(\lambda)$. According to GUM Supplement 1 [6], MCM may be a suitable choice for this uncertainty evaluation.

A method to derive the uncertainty of $S(\lambda)$ was described in [1]. Responsivity measured at 9 wavelengths were firstly fitted to the model in [2] to obtain the uncertainties and correlations of the 4 parameters P_f, T, P_b and D. These uncertainties were then propagated to $S(\lambda)$ using the physical model.

SCL applies MCM to generate random samples for the input quantities, perform model fitting and calculate $S(\lambda)$ in each trial. The uncertainty is obtained by summing up the results from a large number of trials. In the past, SCL had developed a software tool in Visual C and Visual Basic for Application (VBA) with Microsoft Excel as frontend user interface to evaluate uncertainties using MCM. This software was adapted for this application. The measurement model is encoded in VBA which includes the NM algorithm and equations (1) to (4). The values of S_i are entered in an Excel worksheet with an example shown in Table 1. They are taken to have Gaussian probability density function (pdf) with relative standard uncertainty of 0.03 % (converted to absolute values in the table). Since these data were measured by the same cryogenic radiometer, they are correlated and the correlations should be considered in the uncertainty evaluation [1]. It is estimated that the correlation coefficient between them is 0.5. A method to generate multivariate Gaussian distribution is described in section 6.4.8 of [6].

λ	pdf *	value	std uncert	Correlation Coefficient						
406.7	G	0.319342	0.000096	1	0.5	0.5	0.5	0.5	0.5	0.5
413.1	G	0.325138	0.000098		1	0.5	0.5	0.5	0.5	0.5
476.2	G	0.380091	0.000114			1	0.5	0.5	0.5	0.5
530.9	G	0.425322	0.000128				1	0.5	0.5	0.5
568.2	G	0.455770	0.000137					1	0.5	0.5
647.1	G	0.519709	0.000156						1	0.5
799.3	G	0.642299	0.000193							1

*G=Gaussian

Table 1. An example of input quantities

Since the responsivity model is non-linear, the user might need to experiment with the starting values of the NM algorithm to achieve good results. It will be a good idea to view the distribution of the fitted parameters to judge if the fitting has worked well. An example of the pdf of the P_f parameter after 100000 MCM trials is shown in Figure 1(a).

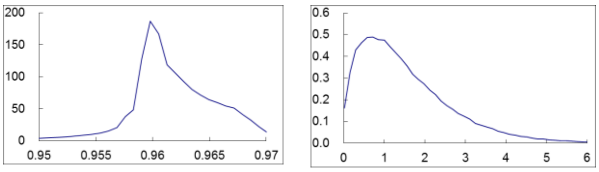

Figure 1. (a) pdf of P_f , (b) Histogram of χ^2

RESULTS AND DISCUSSIONS

Model fitting will not be perfect. There will be residual error in each fitting. The χ^2 parameter defined below can be used to assess the goodness of fit [1]. M is a vector of the fitting errors ($S(\lambda) - S_i$). U_x is the variance covariance matrix of the input quantities. N and P are the number of inputs and fitting parameters. The χ^2 varies vastly for different MCM trials. The histogram of χ^2 for 100000 MCM trials is shown in Figure 1(b)

$$\chi^2 = M^T {U_x}^{-1} M/(N-P) \qquad (6)$$

The residual should be included in the uncertainty of $S(\lambda)$. Different ways to handle this component will have great impact on the reported uncertainty as depicted in the MCM computation results shown in Figure 2. The dots E indicate the uncertainties of the input quantities to facilitate comparison.

Curve A does not include the uncertainty due to fitting. It indicates the uncertainty of $S(\lambda)$ arising from that of S_i alone. Curve C is obtained by adding to curve A the uncertainty due to individual fitting in each MCM trial. The values are much larger than other curves due to the variation of fitting quality in different MCM trials as shown in Figure 1(b). A possible explanation is that the model might not fit well when random values are added to S_i. Curve C therefore does not represent well the uncertainty of $S(\lambda)$ and should not be used. Curve B is curve A adding a fixed uncertainty component representing the fitting error at S_i. Although the MCM makes a large number of trials, the only set of $S(\lambda)$ that we will use in future work is the set calculated from S_i. Hence curve B is a good representation of the uncertainty of $S(\lambda)$. Curve D is similar to curve A except that the correlations between the input quantities are treated as zero. The result shows the importance of considering the correlations of input quantities.

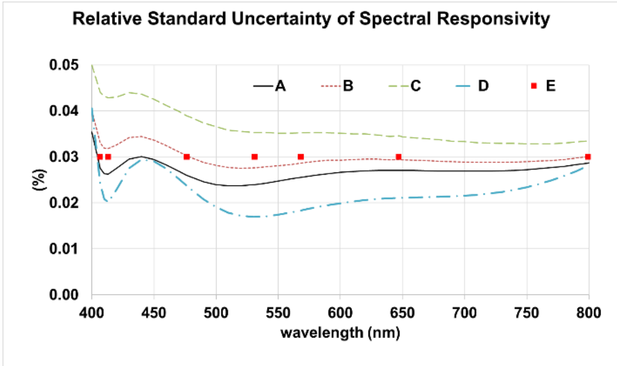

Figure 2. Results of the Monte Carlo computation

CONCLUSION

A procedure for interpolating responsivity and evaluating uncertainty using MCM was described.

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