Optics Communications 475 (2020) 126254

Contents lists available at ScienceDirect

Optics Communications

journal homepage: www.elsevier.com/locate/optcom

Research on the irradiance calibration of a VUV dual-grating spectrometer based on synchrotron radiation

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ARTICLE INFO

Keywords:
Radiometry
High accuracy calibration
Synchrotron radiation
Irradiance
Responsivity
VUV spectrometers
Space instrument

ABSTRACT

A high accuracy instrument calibration is the guarantee of obtaining high precision atmospheric inversion data from a wavelength-dispersive space remote sensing instrument in the orbit. To improve the relative calibration uncertainty of a dual-grating spectrometer in the vacuum-ultraviolet (VUV) band, conventional secondary standard light sources, such as deuterium lamps, used in laboratory calibrating stations are not suited to meet high precision. In this paper we present the calibration of the space instrument based on the Metrology Light Source (MLS) of the Physikalisch-Technische Bundesanstalt (PTB) operated as a primary synchrotron radiation (SR) source with calculable spectral radiant intensity to overcome the limit imposed by secondary transfer standards. For taking into account the difference between the highly linearly polarized SR source and the un-polarized solar radiation, which will be observed by the dual-grating spectrometer in orbit, the calibration was performed at two orientations of the instrument, which are perpendicular to each other with respect to the incident SR. The factors contributing to the uncertainty budget were analyzed. It could be shown that a total relative uncertainty of 2.52% can be achieved, which has greatly improved the calibrating accuracy compared with that obtainable with the conventional standard light source calibrating stations in the VUV spectral range.

1. Introduction

Solar spectrometers are usually adopted to monitor the variation of the solar activity. Since the 1970s, Solar Backscatter Ultraviolet Spectrometer (SBUV) [1], Solar Ultraviolet Spectral Irradiance Monitor (SUSIM) [2], SOLar-Stellar Irradiance Comparison Experiment (SOLSTICE) [3,4], Solar Irradiance Monitor (SIM) [5] and Solar Spectrum (SOLSPEC) [6] were in succession developed and successfully used for in orbit long-term monitoring of solar spectral irradiance. A great deal of valuable information about the solar activity and its long-term change are achieved.

With the in-depth development of space remote sensing technology and the increasing demand for quantitative application of remote sensing products, the high accuracy calibration of space remote sensing instrument is particularly important. Based on the characteristics of the VUV dual-grating spectrometer observation target in orbit, i.e. to detect slight variations in solar activity, the VUV dual-grating spectrometer must operate with of high precision and high accuracy in the orbit. However, a high accuracy calibration is the necessary prerequisite for a high-accuracy traceable measurement with the spectrometer, which we focus on in this paper.

Under normal conditions, the relative uncertainty based on a deuterium lamp transfer standard in the VUV is typically more than 7%, which cannot meet the high accuracy requirement of monitoring solar activity. However, a SR source with the appropriate instrumentation to measure the storage ring parameters can be operated as a primary source standard, the spectral radiant intensity of which can be calculated with high accuracy from the VIS to the X-ray region [7,8]. Moreover, SR sources have high stability and reproducibly and the spectral radiant intensity can be adjusted by an appropriate choice of the electron beam current. So a direct calibration of the space instrument to an electron storage ring as a primary source, and thus preventing the detour of using a transfer standard, can considerably improve the calibration accuracy. Because of the highly linearly polarized SR, the calibration has to be performed under two orientations with

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https://doi.org/10.1016/j.optcom.2020.126254
Received 3 May 2020; Received in revised form 15 June 2020; Accepted 6 July 2020
Available online 8 July 2020

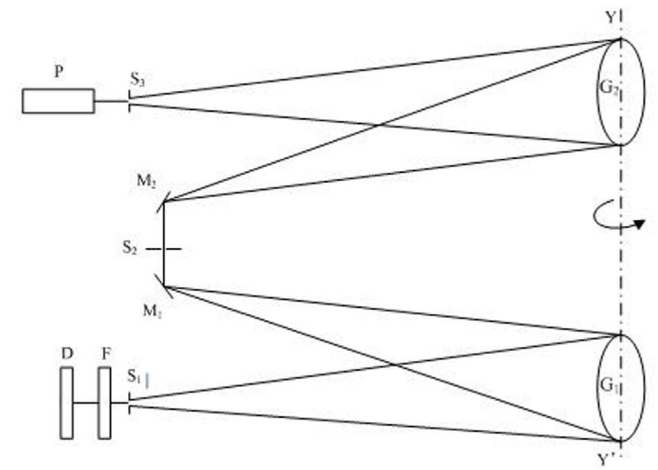

Fig. 1. The structure of dual-grating spectrometer.
D: Diffusor Transmission Plate F: Filter P: Photomultiplier Tube S_1: Entrance Slit G_1: Grating 1 M_1: Mirror 1 S_2: Middle Slit G_2: Grating 2 M_2: Mirror 2 S_3: Exit Slit.

respect to the axis of the incident radiation, which are perpendicular to each other, to exclude effects caused by the polarization ability of the measured instrument.

Since the SR was used in spectroscopy [9], the SR based radiometry work of National Institute of Standards and Technology (NIST) and Physikalisch-Technische Bundesanstalt (PTB) are currently the most representative ones [10]. NIST has built the SURF-I, SURF-II and SURF-IIISR sources, which have been used for the calibration of multiple space remote sensing instruments in VUV band [11]. The PTB started SR based radiometry at the now-closed BESSY I electron storage ring focusing on fundamental radiometry and the realization of transfer standards, mainly by using deuterium lamps with MgF_2 window from 116 nm to 400 nm. Subsequently, the PTB uses the SR source BESSY II to extend the calibration spectrum to the X-ray spectral range [12,13].

The PTB synchrotron radiation source Metrology Light Source (MLS) was built in 2008, which is presently the largest and most advanced SR source dedicated to metrology. The intensity of the radiation can be changed by selecting the number of stored electrons, the electron energy can be set between 105 MeV and 630 MeV, and the characteristic wavelength of the radiation is thus altered over the wide range from 735 nm to 3.4 nm [14].

2. Experimental set-up and calibration principle

2.1. The structure of the dual-grating spectrometer

The structure of the dual-grating spectrometer is shown in Fig. 1. It consists of a diffusor transmission plate D(fused-silica materials), an optical filter F, an entrance slit S_1, a middle slit S_2, an exit slit S_3, two plane mirrors M_1 and M_2, two concave gratings G_1 and G_2 with a grating line density of 3600 lines/mm and a photomultiplier tube P(MgF_2 window) operating in photon counting mode. The two gratings simultaneously rotate round the YY′ axis, driven by stepper motors to cover the spectral range from 165 nm to 320 nm. The surface of the two plane mirrors and the two concave gratings are Al coated with a MgF_2 topping layer for high reflectivity in the UV band. Spectral resolution is 1 nm, wavelength repeatability is 0.01 nm, wavelength precision is less than 0.05 nm.

The solar radiation irradiates the pre-diffuser of VUV dual-grating spectrometer following the normal direction of the pre-diffuser, and finally forms a spectral image of the entrance slit on the plane of the exit slit. The stepping motor under the control of the computer synchronously rotates the two gratings through sinusoidal mechanism and executes the spectral scanning. The monochromatic radiation with different wavelength in succession is detected by the photomultiplier which finally form a solar spectrum.

2.2. Set-up at the beamline

Diagram of synchrotron radiation MLS calibrating spectrometer is shown in Fig. 2.

For the calibration at the MLS, the VUV dual-grating spectrometer has been mounted into a vacuum chamber that was placed on an adjustable platform at the end of the MLS white light beamline at a distance of 21.722 m from the SR source point. The respective electronic box was operated in a separated vacuum chamber that was connected to the vacuum chamber containing the spectrometer by means of a below which also accommodated the harness. To take account of the highly polarized SR, see Fig. 3, the instrument had to be measured at two orientations, which are perpendicular to each other.

To change the instrument orientation, the vacuum chamber had to be vented. The white light beamline is equipped with a guiding laser that can be superimposed to the SR beam by means of a pellicle that can be temporary introduced into the optical path for alignment purpose. The guiding laser has been aligned prior to the calibration measurement and defines in the vertical direction accurately the orbital plane of the SR and in the horizontal direction approximately the center of the white light beamline. For the calibration the SR was confined by computer controlled aperture plates to slightly overfill the diffusor plate D. Because the vacuum that was achievable in the chamber containing the spectrometer did not match the requirements necessary to open the beamline towards the electron storage ring, the two vacuum sections were separated by a sapphire window. The transmittance of this window has been characterized, but the related uncertainty of the transmittance measurement is not included in the uncertainty budget of this proof of principle experiment since it can be avoided in principle.

2.3. Calibrating principle of synchrotron radiation

The dual-grating spectrometer in orbit will observe the un-polarized solar radiation, while the SR used for calibration is highly linearly polarized. To reduce the influence of the two different polarization states on the spectrometer response, the method of rotating calibration has been applied, that is, the spectrometer was placed in the horizontal and the vertical direction, respectively, to obtain the responsivity of the two directions. Finally, according to the superposition principle of polarized light, the irradiance responsivity of the spectrometer to un-polarized solar radiation is the mean value of 0° polarization responsivity and 90° polarization responsivity [15,16]. The details are as follows:

The initial orientation of the spectrometer was placed horizontally (0° polarization direction). The spectral irradiance of the synchrotron radiation source $E(\lambda)$, then leads to the output signal $S_1(\lambda)$ of the spectrometer, and the irradiance responsivity of the spectrometer, $R_1(\lambda)$, can be expressed as follows:

$$R_1(\lambda) = \frac{S_1(\lambda)}{E(\lambda)} \tag{1}$$

Rotating the spectrometer 90° vertically, the spectral irradiance of the SR source is still $E(\lambda)$. The output signal of the spectrometer is then $S_2(\lambda)$ and the irradiance responsivity of the spectrometer, $R_2(\lambda)$, can be expressed as follows:

$$R_2(\lambda) = \frac{S_2(\lambda)}{E(\lambda)} \tag{2}$$

Then, the spectral irradiance responsivity for un-polarized radiation of the spectrometer is given by

$$R(\lambda) = \frac{R_1(\lambda) + R_2(\lambda)}{2} \tag{3}$$

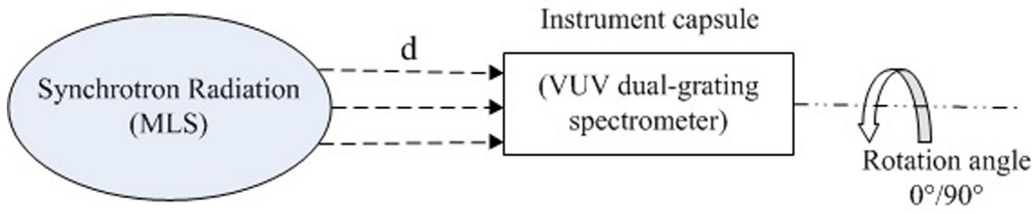

Fig. 2. Diagram of synchrotron radiation MLS calibrating spectrometer.

Table 1
Measured response signal of the VUV dual-grating spectrometer for selected wavelengths normalized to 1 mA.

Wavelength/nm	0°polarization/counts s^{-1}	90°polarization/counts s^{-1}
165	1.446	3.274
180	4.109	8.966
195	9.056	13.777
210	15.986	15.600
225	22.145	16.260
240	20.582	19.317
255	10.418	12.394
270	10.964	7.626
285	5.610	4.434
300	1.400	1.367
315	0.205	0.220

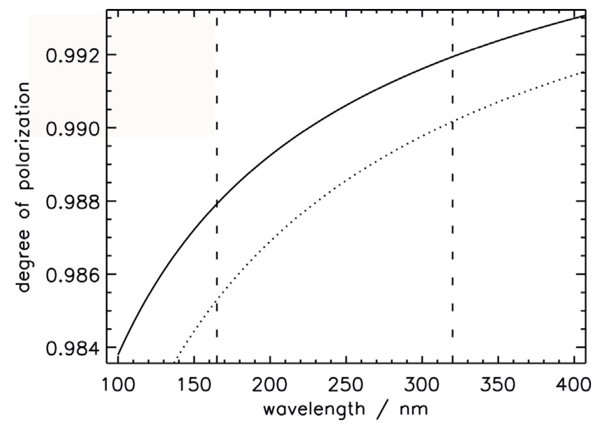

Fig. 3. Degree of polarization of the synchrotron radiation in the spectral range of the spectrometer (marked by two vertical dashed lines) in an aperture of 8 mm (h) ×12 mm (v) at a distance of 22 m. The solid line gives the degree of polarization for the aperture centered exactly on the orbital plane, the dotted curves, for the aperture with a 2 mm vertical offset due to a possible misalignment.

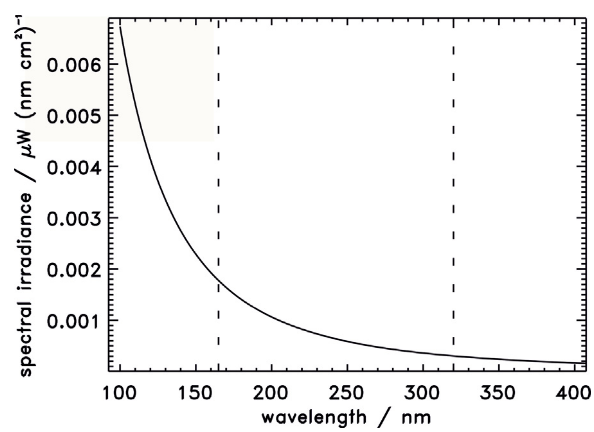

Fig. 4. Calculated spectral irradiance of the synchrotron radiation incident onto the spectrometer diffusor for an electron beam current of 1 mA.

3. Synchrotron radiation calibration

3.1. Synchrotron radiation calibrating process

After the instrument was mounted in the vacuum chamber in the desired orientation, it was aligned in such a way the beamline pilot laser was incident onto the center of the diffusor plate. By observation of the laser reflection, the spectrometers pitch and azimuth angles were aligned to normal incidence. After alignment, the vacuum chamber was closed and pumped down. Once a pressure below 6.5×10^{-3} Pa was reached, the built-in mercury lamp (with characteristic spectral lines at 184.892 nm, 253.652 nm and 296.728 nm) was used for an initial system test and spectral pre-calibration. Moreover, the wavelength position accuracy and the status of the spectrometer were confirmed. Thereafter the photo shutter of the white light beamline was opened so that the highly polarized SR is incident onto the spectrometer. According to the intensity of the SR source and the response signal of the spectrometer, a stable signal output was ensured by adjusting the integrating time of photomultiplier electronics. After half an hour of warm-up of the spectrometer, the calibration measurement was performed and repeated two more times. After closing the beamline's photon shutter, the measurements with the built-in mercury lamp are again performed to confirm the wavelength position accuracy and the instrument status. Thereafter, the system was vented and the spectrometer mounted in the next orientation, perpendicular to the previous one, and the above described measurement procedure was repeated.

3.2. Synchrotron radiation calibration results

The calculated spectral irradiance of the SR that is incident onto the spectrometer's diffusor plate is shown in Fig. 4 for the wavelength range of the spectrometer from 165 nm to 320 nm. The calculated data values are for an electron beam current of 1 mA. The actual measurements have been performed with electron beam currents decaying between 140 mA and 80 mA. The measured response signal of the spectrometer, i.e., the count rate of the photomultiplier normalized to an electron beam current of 1 mA, is given in Table 1 for selected wavelengths.

The responsivity of the spectrometer, calculated according Eqs. (1)–(3) are presented in Fig. 5 for the two different incident polarizations and the mean value. The response for the two polarization directions differ considerably, which is mainly caused by the response of concave grating to different polarized light, still present after passing the diffusor. The basic material of the diffusor plate is high grade radiation-hardened fused silica, and the preparation process mainly adopts a physical grinding method. An ideal diffusor plate would homogenize the incident light and would eliminate polarization. However, laboratory experiment results show that the diffusor cannot completely eliminate the polarization, even if two or more diffusor plates are used. Therefore, the rotating calibration method is adopted to reduce the influence of the different polarization states of the light sources (the on-orbit light source is the sun and the high accuracy calibration source is SR) on the instrument response during the process of the calibration with SR.

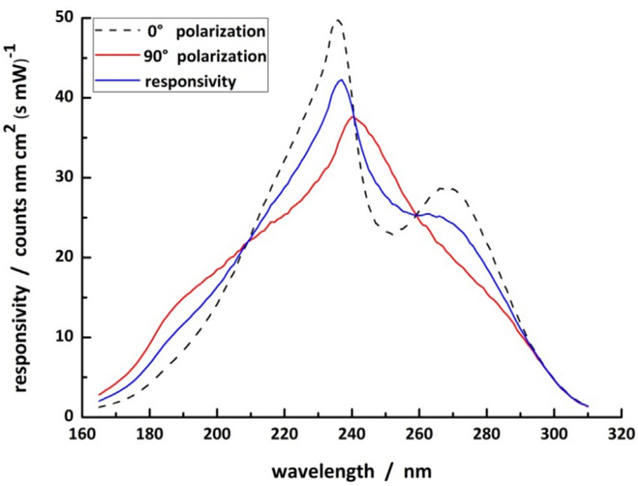

Fig. 5. Spectral irradiance responsivity curves of the dual-grating spectrometer.

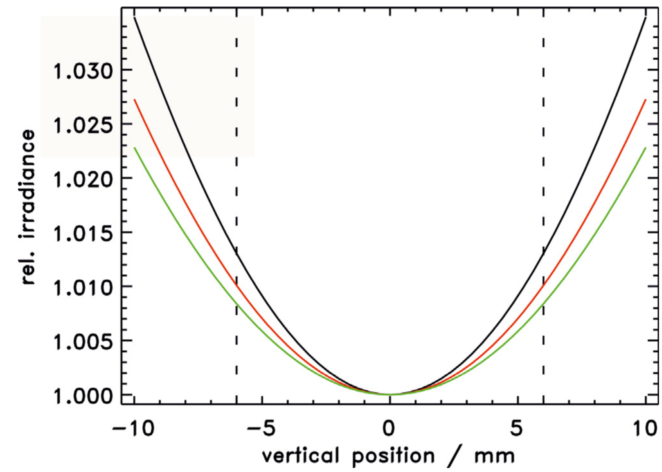

Fig. 6. Relative vertical irradiance distribution of the SR for some wavelengths (165 nm (green), 215 nm (red) and 265 nm (black)).. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

4. Uncertainty budget

The uncertainty contributions are mainly divided into three categories: the SR source uncertainty, the uncertainty introduced by the calibrating process as well as the uncertainty introduced by spectrometer self-measurement. The uncertainty introduced by the calculation of the SR from the MLS electron storage ring is given by the uncertainty of the storage ring parameters. The uncertainty introduced in calibrating process includes the measurement error of the distance and alignment errors of the instrument with respect to the incident beam. The spectrometer self-measurement uncertainty includes self-measurement repeatability, the wavelength offset and nonlinear effects.

The contributions to the uncertainty budget are described below in detail.

(1) Uncertainty in the SR calculation

SR is used as primary source radiation with high precision. If the relevant parameters of the SR source, the electron beam energy, the magnetic induction of the bending magnet at the radiation source point, the electron beam current and the electron beam source size and divergence are determined, the spectral radiant intensity of the SR can be calculated by the Schwinger formula. The uncertainty of the calculation is determined by the uncertainty in the measurement of these parameters. Details of the calculation of the spectral radiant intensity and the measurement of the storage ring parameters can be obtained [8].

The spectrometer, as described in this paper, operates in the wavelength range from 165 nm to 320 nm, i.e. in the photon energy range from 7.45 eV to 2.73 eV ($E = h\nu = h\lambda/c$). In this spectral range the relative uncertainty in the calibration of the spectral radiant intensity, without an explicit high-accuracy measurement of the above listed parameters, is below 0.1% [17].

(2) Corrected residual uncertainty of the decaying electron beam current

The SR intensity gradually decays over time because of the finite lifetime of the stored electron beam. The measurement signal can be normalized to the electron beam current, which is monitored by PTB at each moment with high accuracy [8]. However, the scanning time and reset time of the motor leadscrew driving the grating angle cannot be accurately obtained in the process of spectrometer signal acquisition, which leads to a certain contribution to the uncertainty budget. According to the start and the end time of each measurement recording in the calibration process and the monitoring of the electron current, the duration of each measurement is 10 min. The SR intensity decreases by 2.1% during this measurement time, so the SR intensity attenuation rate is about 0.21%/min. The maximum time error of each calibration is estimated to be about 20 s by driving the motor leadscrew and setting the integration time. Therefore, the modified residual uncertainty of energy attenuation of SR is 0.07%.

(3) Measurement uncertainty of the calibration distance

Electron storage rings are primary source standards for spectral radiant intensity. The spectral irradiance was calculated be divided the spectral radiant intensity by the square of the distance from the source point to the diffusor plate. This is valid because of the point-like source of the SR and the large distance from the source to the instrument. The distance was determined to be (21 722 ± 10) mm which leads to a contribution to the relative uncertainty of 0.09%. The uncertainty formula is shown in the relation (4).

$$U_{\_distance} = (1 - \frac{(d-d')^2}{d^2}) \times 100\% \quad (4)$$

(4) Optical axis parallelism alignment error

The diffusor plate, made off used quartz, which homogenizes incident light, can be regarded as an ideal lambert body within a small angle range of ±3°. Complying with Lambert's law of cosines, which states that the intensity of light diffused in all directions is proportional to the $\cos\theta$(θ is between the incident light and its normal). In the case of normal-incidence $\cos\theta = 1$. In the worst case for the adjustment of optical axis parallelism, the aligned error of two optical axes is equal to $\theta' = 0.8°$. The uncertainty formula is shown in the relation (5). Therefore, the uncertainty $U_{\_axis}$ introduced by optic axis alignment is 0.01%.

$$U_{\_axis} = \left|\frac{\cos\theta' - \cos\theta}{\cos\theta}\right| \times 100\% \quad (5)$$

(5) Vertical alignment error

Despite the laser-aided alignment, a possible vertical alignment error is included into the uncertainty budget. The vertical distribution of the SR irradiance is not completely uniform as can be seen from Fig. 6. Estimating 2 mm as a maximum possible vertical alignment offset would result in a 0.2% change in the spectral irradiance.

(6) Rotation angle alignment error

The instrument had to be measured under two orientations which are perpendicular to each other. As a reference, the bottom plate and the side plate of the spectrometer box are used. A maximum possible deviation from perpendicularity for these plates of 0.5° is estimated, resulting in a relative uncertainty of 0.9%.

(7) Spectrometer self-measurement repeatability

The repeatability of the spectrometer self-measurement is related to the output signal of the spectrometer. The output signal data is

Table 2
Uncertainty analysis of calibration with SR.

Source of uncertainty	Rel. uncertainty value
Spectral radiant intensity of the SR calibration	0.10%
Corrected residual uncertainty of the decaying electron beam current	0.07%
Measurement uncertainty of the calibration distance	0.09%
Optical axis parallelism alignment error	0.01%
Optical axis center alignment error	0.20%
Rotation angle alignment error	0.90%
Spectrometer self-measurement repeatability	2.10%
Spectrometer wavelength offset	0.90%
Spectrometer self-nonlinearity	0.50%
Total uncertainty	2.52%

shown in Table 1. The data of the 165 nm band, which has the worst repeatability, was taken as the upper limit, resulting in relative uncertainty contribution of 2.1%.

(8) Wavelength offset

To monitor the wavelength offset caused by a temperature rise during the calibration, the characteristic spectral lines of the built-in mercury lamp were measured at the beginning and at the end of calibration. The maximum wavelength offset between the start and the end of the monitoring test was 0.03 nm. According to the response signal of the spectrometer, the maximum radiation signal offset introduced by a 0.03 nm wavelength offset is 0.9%.

(9) Spectrometer self-nonlinearity

The residual nonlinear error of spectrometer is less than 0.5%, which is based on the maximum count rate of the spectrometer output signal and the non-linearity test results in the laboratory.

The contributions to the relative uncertainty in the calibration of the spectrometer with SR at the MLS electron storage of the PTB are summarized in Table 2. Since the uncertainties are not correlated, the total standard uncertainty is given by the equation (6) of uncertainty propagation.

$$u_e = [\sum_{i=1}^{N} u^2\left(x_i\right)]^{1/2} \tag{6}$$

In the formula (6) u_e is total uncertainty, N is the number of uncertainty sources, $u\left(x_i\right)$ is the source of each uncertainty. The total uncertainty adds up to 2.52%.

As mentioned above, not included is the transmittance of the sapphire window used to separate the vacuum section, because this will be obsolete if a better vacuum can be reached for the spectrometer. Typical uncertainty values for the transmittance measurement and homogeneity of the window within the illuminated area would contribute with about 1% to the uncertainty budget. Also not included are possible degradation effects of the optical components which can be substantial in this spectral range.

5. Conclusion

To improve the quality of inversion data, an accurate absolute radiometric calibration of the remote sensing instrument in orbit is necessary. Normally, in the spectral range mentioned in this paper, the calibration is performed by transfer sources which previously have been calibrated traceable to a primary standard. Often used and rather easy to handle transfer sources in the UV/VUV spectral range are D2 lamps. Using a transfer source usually increases the calibration uncertainty because of an additional calibration step and the limits given by the stability and reproducibility of the transfer source itself. In this proof-of-principle experiment a direct calibration of the space instrument to a primary source standard, the MLS electron storage ring with calculable SR, was performed. The potential of this method has been proven by pushing the total relative uncertainty of the calibration well below of 2.52% which cannot be obtained by a calibration via transfer sources.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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