Polarization properties and microfacet-based modelling of white, grey and coloured matte diffuse reflection standards

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Abstract. To elucidate the influence of polarization in diffuse reflectometry, we performed a series of measurements in several bidirectional geometries and determined the Stokes parameters of the diffusely reflected radiation. Different types of matte reflection standards were used, including several common white standards and ceramic colour standards. The dependence of the polarization on the sample type, wavelength and geometry have been studied systematically, the main influence factors have been identified: The effect is largest at large angles of incidence or detection and at wavelengths where the magnitude of the reflectance is small. The results for the colour standards have been modelled using a microfacet-based reflection theory which is derived from the well-known model of Torrance and Sparrow. Although the theory is very simple and only has three free parameters, the agreement with the measured data is very good, all essential features of the data can be reproduced by the model.

1. Motivation
To obtain accurate and reliable results in diffuse-reflectometry experiments, one has to take all possible factors into account that have an impact on the experiment. One such factor on which we focus here is polarization. The polarization-related properties of the measurement apparatus as well as those of the sample under test have to be considered.

PTB’s gonioreflectometer [1] has been equipped with a polarization-analyzer unit which allows to determine the Stokes parameters of the detected radiation [2]. We conducted a series of experiments to determine the main polarization dependence and influence factors and modelled the data.

2. Experimental details
The spectral radiance factor \( \beta \) of different reflection standards was determined using PTB’s gonioreflectometer. A detailed description of the apparatus and the measurement procedure can be found in [1].

2.1. Matte diffuse-reflection standards
Various types of samples have been examined, among them some of the most common types of reflection standards. All samples had a diameter of 50 mm and a matte surface finish. Three different types of white reflection standards have been used: Opal glass, barium sulfate and ceramic. The spectral dependence of the polarization properties was examined using a set of coloured ceramic reflection
standards (light grey, dark grey, red, green and blue) within a comparison carried out in the project xDReflect [3]. Sandblasted aluminum was also investigated as a sample without sub-surface scattering contribution.

2.2. Stokes parameters and measurement procedure
A polarization-analyzer unit has been used to determine the Stokes parameters of the radiation, details of the setup and the measurement procedure can be found in [2]. The four Stokes parameters describe the polarization in terms of total intensity (I), linear polarization at 0°/90° orientation (M₀), linear polarization at +/-45° orientation (C₀) to the scattering plane, and circular polarization (S₀). The subscript “0” indicates that they are normalized by the intensity and converted to percent. The degree of polarization DOP is given by DOP = √M₀² + C₀² + S₀². Since the light source used in the experiment is completely unpolarized, any detected polarization must originate from the sample under test.

For the measurements presented here, the geometry of illumination and detection has been varied (e.g. angle of incidence 𝜃𝑖 was kept constant at 0° while the angle of detection 𝜃𝑟 has been varied up to +/-75° in steps of 15° or vice versa. 𝜃𝑖/𝑟 > 0 means that the angle is measured from the surface normal (z-axis) in the direction of the positive x-axis, for 𝜃𝑖/𝑟 < 0 it is measured in the direction of the negative x-axis). The measurements were carried out at several fixed wavelengths in the visible spectral range.

3. Microfacet-based modelling
Data in this work has been described by the reflection model of Torrance and Sparrow [4]. It assumes that a rough surface is composed of mirror-like facets that have a distribution of slopes. There are two contributions to the reflected radiation. First, a specular contribution which is caused by specular reflection off those microfacets which have a suitable orientation. Polarization is included by using the Fresnel reflection coefficients to calculate the specular contribution. And second, a diffuse contribution which is assumed to be perfectly Lambertian.

The Torrance—Sparrow model shows a reasonable agreement with the measured data for most data sets, but it systematically fails if β_p > β_s (β_s/p: spectral radiance factor for unpolarized incident radiation and detection sensitive only to s- or p-polarization, respectively). Thus, we decided to modify the Torrance—Sparrow model by coupling the specular and diffuse contributions. A similar approach has been used by Shirley [5], based on the idea that the diffuse contribution is modified to account for “specular losses”: Any fraction of radiation, that has been reflected specularly, cannot contribute to the diffuse reflection. So, the diffuse contribution has to be decreased by the amount of specular reflection.

Since we found that for in-plane measurements only M₀ contributes to the state of polarization, it is sufficient to consider the radiance factor for s and p polarization, given by

\[ \beta_s/p = \beta_s/p, \text{specular} + \beta_s/p, \text{diffuse} \]

\[ = b R_s/p(n_1, n_2, \theta_i, \theta_r) G(\theta_r) P(\theta_i, \theta_r) + a\cos \theta_i \left(1 - R_s/p(n_1, n_2, \theta_i, \theta_r)\right) \]

where \( R_s/p(n_1, n_2, \theta_i, \theta_r) \) are the Fresnel reflection coefficients for s and p polarized radiation. \( G(\theta_r) \) is a shadowing function that accounts for masking and shadowing of the facets. In the original publication by Torrance and Sparrow, it is derived based purely on geometric optics. This results in a piecewise definition of \( G \), which leads to discontinuities when fitting our data. Instead, we used a very simple, more empirical expression for \( G(\theta_r) \), given by

\[ G(\theta_r) = \frac{4}{\pi^2} \left(-\theta_r^2 + \frac{n^2}{4}\right) \]

\[ P(\theta_i, \theta_r) \] is the facet distribution which is assumed to be Gaussian

\[ P(\theta_i, \theta_r) = \exp \left(-c^2 \cdot \left(\frac{\theta_i - \theta_r}{\frac{\pi}{2}}\right)^2\right) \]
The explicit wavelength dependence of the refractive indices and of the spectral radiance factor are omitted in this notation for better readability. To fit the model and to visualize the measured data in a less complex form, we used the ratio $\beta_{\text{ratio}} = \frac{\beta_s}{\beta_p}$ vs the angle $\theta_{i/r}$. The ratio makes it easier to identify small polarization effects ($\beta_{\text{ratio}} \approx 1$) compared to $\beta_s$ and $\beta_p$. The refractive index of air was assumed to be unity ($n_1 = 1$). The refractive index of the ceramic reflection standards was determined by MSL, yielding values between 1.49 and 1.53. To model the data, we used a value of $n_2 = 1.5$. In this way, there are only three free parameters left for fitting: the relative amplitudes $a$ and $b$, and the inverse width $c$ of the facet distribution.

4. Results and discussion

4.1. Material dependence of polarization properties

Matte white standards are one of the most important classes of artefacts in diffuse reflectometry. They are used as reference artefacts in many applications. Thus, characterizing their polarization properties is of paramount importance. There are two mainly used bidirectional geometries in diffuse reflectometry of white standards. Either the radiation is incident perpendicular to the sample surface and detection takes place under 45° ($\theta_i = 0^\circ, \theta_r = 45^\circ$, denoted $0^\circ:45^\circ$), or vice versa ($\theta_i = 45^\circ, \theta_r = 0^\circ$, denoted $45^\circ:0^\circ$).

| Sample type   | geometry  | $M_0$ / % |
|---------------|-----------|-----------|
| Barium sulphate | $0^\circ:45^\circ$ | -0.65     |
| Barium sulphate | $45^\circ:0^\circ$ | -1.23    |
| Opal glass    | $0^\circ:45^\circ$ | 2.7      |
| Opal glass    | $45^\circ:0^\circ$ | -0.97    |
| Ceramic       | $0^\circ:45^\circ$ | 0.90     |
| Ceramic       | $45^\circ:0^\circ$ | -1.48    |

All white standards that have been studied in this work exhibit a small, but non-zero amount of linear polarization that is introduced by reflection. The amount of linear polarization gets larger if either angle is increased. This effect is most pronounced for Opal glass. Even at $0^\circ:45^\circ$, $M_0$ already has a value of about 3%, increasing up to 10% at $\theta_r = 75^\circ$. For barium sulfate, $M_0$ is well below 4%, for ceramic even below 2%, even at large angles. The values obtained for both are summarized in Table 1. Measurements for Opal glass and ceramic were carried out at 700 nm, measurements for barium sulphate at 750 nm.

It was shown that for Opal glass at large detection angles, the reflected radiation is clearly partly polarized. The degree of polarization can become fairly large so that this effect cannot be neglected.

4.2. Spectral dependence of polarization properties

The wavelength dependence of the spectral radiance factor of the six ceramic standards (white, light grey, dark grey, red, blue and green) has been measured in a polarization-resolved way at MSL in the wavelength range between 370 nm and 720 nm. This allows to calculate the ratio $\beta_{\text{ratio}}$ for the entire visible spectral range. The spectral measurements were carried out in both the geometries $0^\circ:45^\circ$ and $45^\circ:0^\circ$. The results for all six standards are shown in Figure 1. The ratio $\beta_{\text{ratio}}$ is plotted against the radiance factor for the unpolarized case, $\beta_{\text{unpol}}$, which is calculated as the average of the radiance factors for $s$ and $p$ polarization.
Figure 1. Spectral radiance factor ratio for all six ceramic reflection standards.

A strong correlation between the reflectance (given by the magnitude of $\beta_{\text{unpol}}$) and the polarization dependence can be seen: The lower the reflectance, the higher the ratio $\beta_{\text{ratio}}$, i.e. the larger the degree of polarization. This kind of observation has also been reported in other fields of reflectometry [6].

So, for this type of ceramic reflection standards, the reflectance indicates how large the influence of polarization is. For light samples and in the maxima of the reflection spectra, only a small influence can be expected. However, for dark samples and in the minima of the spectra, the influence can become very large, as ratios $\beta_{\text{ratio}}$ up to 1.45 have been observed.

4.3. Geometry dependence of polarization properties

Since we have seen that for white standards, the measurements geometry plays a vital role for the polarization, we studied the influence of the geometry for the ceramic coloured standards as described in section 1.3. As for the white standards, we found that for larger angles, the influence of polarization increases. However, depending on the sample and the wavelength, the DOP gets considerably larger than for white standards. Values of up to 20% were found, especially for the dark samples. It was also observed that for most data sets, $\beta_{\text{ratio}} > 1$. For the white and red samples at large detection angles, we found $\beta_{\text{ratio}} < 1$. Some exemplary data sets are shown in Figure 2, together with the fit curves from the microfacet-based reflection model. It is apparent that there is a good qualitative agreement between the experimental data and the fit. All essential features of the data are well reproduced by the microfacet model. Although the agreement between the data and the model is remarkably good, considering that the model is very simple and only has three free fitting parameters, there are some shortcomings. They can be seen most clearly when we illustrate the dependence of the fit parameters on the magnitude of the DOP. The amplitude $b$ of the specular term is almost constant for all data sets and does not depend on the DOP, so we refrain from depicting it graphically. The dependence of $a$ (circles) and $c$ (squares) is shown in Figure 3. Each symbol represents the fit parameter for a trace as given in Figure 2. The colour indicates the colour of the sample, the measurement wavelengths are stated explicitly next to the symbols.
Figure 2. Spectral radiance factor ratio for different geometries. The experimental data are shown together with the best fit results of the microfacet-based reflection model.

The amplitude $a$ of the diffuse contribution clearly decreases as the magnitude of the DOP increases. The higher the DOP, the smaller is the contribution of purely diffusely reflected radiation. It is, however, unexpected to see that the inverse width $c$ of the facet distribution clearly correlates with the DOP. The larger the DOP, the larger $c$ gets. This indicates the oversimplification of the model. At first glance, one would expect $c$ to remain constant, since it is a parameter that describes the geometric characteristics of the reflecting surface. Even though different samples have been used, they are all comprised of the same ceramic and only differ in the dye used to set the color. Thus a similar surface characteristic for all samples can be assumed. It has been shown, though, that it can be useful to work with an “effective” surface parameter which depends on the measurement geometry. He et al. [7] used an effective surface roughness in their model since the roughness appears to decrease for oblique angles due to shadowing of the facets. The wavelength also appears to have an influence on $c$. The scattering behavior depends on the size of the surface structure relative to the wavelength. This is also included in He’s model [7]. This approach has not been pursued in the model presented here, which could at least partly explain the variation of $c$.

Another reason might be that our model is based purely on geometrical optics. Scattering of radiation from a rough surface is a far more complex process, effects like interference on small-scale roughness...
or subsurface scattering can play an important role. None of these are included in the model used here. We can expect subsurface scattering to have a large impact on the reflection properties of ceramic standards. When measuring a matte sample made of sandblasted aluminum in the same geometries as the ceramic standards, almost no effect of polarization was found ($M_0 < 1\%$ even at large angles). For aluminium, subsurface scattering can be ruled out since the radiation does not penetrate the bulk of the material. In turn, this indicates that the large degree of polarization found for the ceramic standards can be connected to subsurface scattering. It probably originates from scattering at the interface between the coloured glaze layer and the ceramic substrate.

5. Conclusion
In this work, we studied the polarization properties of diffusely reflected radiation of matte diffuse reflection standards, including different types of white and coloured standards. For the ceramic coloured standards, we analysed the wavelength and geometry dependence of the polarization properties. We modelled the data using a microfacet-based reflection model that was derived from the model introduced by Torrance and Sparrow.

Only in-plane geometries have been considered, and we found that the only Stokes parameter for linear polarisation $M_0$ has a measurable value. All white standards we studied showed a small, but nonzero DOP. The effect was most pronounced for Opal glass at large detection angles, yielding values of up to 10\%. For barium sulfate and ceramic, the values are smaller, but in general not negligible. When studying the wavelength dependence of the polarization of the ceramic colour standards, we found a clear correlation between the magnitude of the reflectance and the DOP. The lower the reflectance, the higher the DOP, thus the larger is the influence of polarization. At selected wavelengths, we studied the geometry dependence. The larger the angle which is varied (either incidence or detection), the higher the DOP. In short, for dark samples at oblique angles, the DOP can easily take values of up to 20\%. For light samples at almost perpendicular incidence or detection angle, the impact of polarization is much smaller, but still nonzero.

We modelled the data, using a modified Torrance—Sparrow reflection model, in which the diffuse contribution has been modified to account for “specular losses”. Despite being very simple and only having three free fitting parameters, the model yields a remarkably good agreement with the measured data. However, some shortcomings are apparent since some of the variation in the best fit parameters cannot be explained satisfactorily.

Even for such basic artefacts as matte diffuse reflection standards, the influence of polarization has to be considered carefully, as it depends on a number of parameters: the sample material, the wavelength, the measurement geometry, the polarization properties of the measurement setup and the targeted uncertainty.

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