Use of the surface PSD and incident angle adjustments to investigate near specular scatter from smooth surfaces

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ABSTRACT

The Rayleigh Rice vector perturbation theory has been successfully used for several decades to relate the surface power spectrum of optically smooth reflectors to the angular resolved scatter resulting from light sources of known wavelength, incident angle and polarization. While measuring low frequency roughness is relatively easy, the corresponding near specular scatter can be difficult to measure. This paper discusses using high incident angle near specular measurements along with profile generated surface power spectrums as a means of checking a near specular scatter requirement. The specification in question, a BRDF of 1.0 sr^{-1} at 2 mrad from the specular direction and at a wavelength of 1μ m, is very difficult to verify by conventional scatter measurements. In fact, it is impractical to directly measure surface scatter from uncoated Zerodur because of its high bulk scatter. This paper presents profilometer and scatterometer data obtained from coated and uncoated flats at several wavelengths and outlines the analysis technique used to check this tight specification.

Keywords: BRDF, near specular scatter, surface power spectrum, Rayleigh Rice, vector perturbation theory, metrology

1. INTRODUCTION

Limiting scattered light in an optical system is often essential but also, most of the time, challenging. Each and every media or surface in the light path is likely to introduce scattered light that will degrade the image quality. This is even more the case when the object is faint relative to its surroundings. This scattered light limitation is particularly important as it applies to the Advanced Technology Solar Telescope (ATST) [1]. A thorough analysis has established that microroughness of the ATST primary mirror is one the main sources of scattered light [2]. Therefore, in order to meet the science requirement for the ATST, it was critical to specify the primary mirror in terms of its scatter function or more precisely, BRDF. Specifically, this 4 m off-axis parabolic mirror, made of Zerodur, has to meet a BRDF of less than 1.0 sr⁻¹ at 2 mrad from the specular direction at a wavelength of 1 μ m.

Several techniques may be used for measuring the BRDF of a surface. However, such a measurement is difficult when it applies to near specular measurements for large optics where the bare glass has a low reflectivity. However, making coated replicas of the mirror's surface would be a risky, time consuming and expensive approach to test the BRDF of this surface. It was therefore crucial to find an alternative method for determining its BRDF at near specular angles.

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Fortunately, when considering optically smooth, clean, first surface mirrors such as the ATST primary, the widely used Rayleigh-Rice vector perturbation theory establishes a one-to-one relationship between the BRDF and the topography of a surface or, to be more specific, its power spectral density (PSD). This relationship is also known as the Golden Rule and is written below for isotropic surfaces (Eq 1.1):

$$BRDF(f) = \frac{16\pi^2}{\lambda^4} \cos \theta_i \cos \theta_s Q PSD_{2D}(f)$$
Equation 1.1

where λ is the wavelength of the incoming light with units of length, θ_i and θ_s the incident and scatter angles; f is the spatial frequency in polar coordinates and is given in inverse unit of length and Q represents a unitless polarization factor. PSD_{2D} is the 2D power spectral density with units of length to the fourth power. We will most typically use μm^4 , but it also common to find the results in Angstroms². μm^2 (10⁸ μm^4).

It is defined as:

$$\text{PSD}_{\text{2D}}(f_x, f_y) = \lim_{\text{Area} \to \infty} \frac{1}{\text{Area}} |\mathcal{F}[Z(x, y)]|^2$$

where Area represents the surface's area considered, Z(x,y) is the surface height fluctuation at each point (x,y) of the surface in unit of length. f_x and f_y are the spatial frequency in x and y in inverse unit of length, $f = \sqrt{f_x^2 + f_y^2}$. \mathcal{F} denotes the Fourier Transform taken of Z(x,y).

As the measurement of low frequency roughness is relatively easy, this approach provides a simple alternative to BRDF measurements for surfaces meeting the Rayleigh-Rice requirements and allows reformulating the ATST BRDF specification in terms of PSD. This term characterizes the surface microroughness.

The ATST primary mirror is a 4 m diameter off-axis parabola, with a 16 m radius of curvature and a 4 m offset from the parent optical axis. In this configuration, the incident light reaches the center of the mirror with an angle of incidence of approximately 14°. Assuming a 1 μ m wavelength with an incident beam of $\theta_i = 14^\circ$ from the normal to the surface at the center of the mirror, and the mirror surface being highly reflective (Q=1), the ATST primary mirror BRDF specification becomes:

$$BRDF(f_{specification} = 2 \text{ cycles/mm}) \le 1.0 \text{ sr}^{-1}$$
 Equation 1.2

From Eq 1.1 we obtain a specification on the mirror surface finish of:

$$PSD(f_{specification} = 2 \text{ cycles/mm}) \le 0.0067 \,\mu\text{m}^4$$
 Equation 1.3

This paper presents diverse measurements put in place to investigate the possibility to check the ATST tight specification. The results obtained confirm the feasibility of using surface PSD to investigate near specular scatter introduced by optically-smooth surfaces. Thus, Section 2 describes the scatterometer used for direct BRDF measurements and presents how the geometry of the instrument was used to achieve near specular scatter measurements; while Section 3 details the MicroFinish Topographer (MFT) [3], a temporal phase shifting interferometer used for profilometric measurements. Data obtained from the two approaches just mentioned, are processed and compared in terms of surface power spectral density (PSD) as presented in Section 4.

2. NEAR SPECULAR DIRECT SCATTER MEASUREMENTS

The difficulty in measuring scatter near the specular beam is separating scatter from the sample (signal) from scatter created by the scatterometer optics (noise). This is typically done by measuring the no sample scatter, called an "instrument signature," and then comparing the measured sample scatter to the signature multiplied by the sample specular reflectance. There is usually an obvious point where the two results separate. This angle depends on both the scatterometer and the sample and typically varies between 0.05 and 3.0 degrees from the center of the specular beam. Instrument signature depends on wavelength and instrument field-of-view as well as the quality of instrument optics [4]. Near specular sample scatter depends on incident angle as well as wavelength and sample scatter characteristics. In this particular case the mirror BRDF specification of 1.0 sr⁻¹ at 2 mrad (0.11°) is similar to the signature of many

scatterometers. Fortunately the sample (but not the signature) dependence on incident angle can help solve this problem for the current situation where scatter is primarily caused by mild surface roughness.

To see how this can be done, consider the incident plane grating equation which relates grating frequency, f, to the wavelength, λ , the incident angle θ_i and the scattering angle θ_s .

$$f = \frac{\sin \theta_s - \sin \theta_i}{\lambda}$$
 Equation 2.1

Substituting in the specification values ($\lambda = 1.0 \ \mu m$, $\theta_s = 0.11 \ deg$, and $\theta_i = 0$) gives a spatial frequency of 1.9 cycles/mm. So the specification is essentially one of limiting roughness having this spatial frequency. Now if the incident angle is increased to 80 degrees at the same wavelength then we see that the same spatial frequency scatters at 80.65 degrees or 0.65 degrees from specular, which is a much easier measurement to separate signal from the instrument signature. The location that a given spatial frequency scatters from specular also depends on wavelength, but changes in wavelength do not offer a big measurement advantage as both scattering angle and the diffraction limited spot size change. As pointed out in the introduction, the Rayleigh Rice vector perturbation theory can be used to account for changes in BRDF with wavelength at a specific spatial frequency.

2.1 Scatterometer description

Scatter measurements were taken on several samples at two wavelengths to illustrate the advantage of incident angle changes. The instrument is a CASI Scatterometer [4] with a sample receiver distance of 294 mm and a small near specular detector aperture of 340 μ m. Laser sources of 488 nm and 633 nm were used for these experiments. Detector step sizes are programmable and can be made as small as 0.01 degrees. Larger detector apertures are used farther from specular and are inserted at programmable locations. The system centers the small aperture on the specular reflection and then takes measurements relative to this location. Signature symmetry is a good indication of correct specular location. System setup and calibration are checked by measuring a diffuse Lambertian sample with a BRDF of 0.32 sr⁻¹.

2.2 Measurement of the Instrument Signature

The CASI instrument signature was measured for two wavelengths $\lambda = 488$ nm and $\lambda = 632.8$ nm as shown in Figure 2.1.



Figure 2.1.Instrument signature measured for two wavelengths ($\lambda_b = 488 \text{ nm}$ and $\lambda_r = 632.8 \text{ nm}$) as a function of polar angles in degrees. The green area indicates the angular region [0-2] mrad from specular.

A slight asymmetry in the measurements taken at positive and negative angles from specular is also observable, and may be due to a slight misalignment in the setup when collecting the data. This is of little consequence as the angle of interest (2 mrad) for ATST-BRDF specification lies in the region where scatter introduced by the instrument signature is prevalent and clearly constitutes a problem for near specular measurements. However, this issue does not exist with a profilometer measurement for BRDF prediction using the Rayleigh-Rice theory. Thus, the MicroFinish topographer, an interferometric microscope was used to investigate the feasibility of measuring near specular scatter.

3. PROFILOMETRIC MEASUREMENTS- MICRO-FINISH TOPOGRAPHER (MFT)

The roughness measurements were made with a temporal phase shifting interferometer called a MicroFinish Topographer (MFT) that used 4Sight [5] software for data capture and analysis. The MFT was used because it is designed to sit directly on the surface being measured and will be used to measure the roughness of the 4 m diameter ATST mirror without having to make replicas. Figure 3.1 shows the MFT as it was used to measure the roughness of an 8.4 m diameter mirror. Because the MFT is supported by the surface being measured, it is largely immune to vibration and once adjusted for piston and tilt, it can be moved to other locations on the surface without having to make further adjustments to piston and tilt. Other than the mechanical design feature of sitting on the surface being measured, the MFT is a conventional surface roughness interferometer that uses commercial interferometric objectives, a Kohler illumination system with a red LED and a CCD camera.



Figure 3.1- MFT picture measuring the surface topography of one of GMT's (8.4 m in diameter) mirrors

The MFT allows accurate roughness measurements on a wide range of spatial frequencies [6] and, in particular, at spatial frequencies corresponding to near specular directions. Therefore, as shown in the next section, it is possible to use profilometric measurements to predict near specular scatter of smooth surfaces when the corresponding scatter measurement is usually limited by the scatterometer instrument signature.

4. RESULTS

Both scatter and surface measurements were taken on two isotropic surfaces meeting the Rayleigh-Rice requirements: a Silicon wafer as well as a Zerodur optical flat partially coated. The results from those two approaches were then compared in terms of PSD on a logarithmic scale.

The PSD from surface topography measurements (PSD_{surface}) is calculated following the steps below [4] [7]:

- 1. Measurement of Z(x,y) representing the surface topography with piston, tip/tilt and power removed. The p_x , p_y are the pixel sizes in x and y directions. N_x , N_y are the surface map sizes in terms of pixels in x and y directions
- 2. Calculation of PSD_{2D} such that: $PSD_{2D}(fx, fy) = \frac{p_x p_y}{N_x N_y} |FFT_{2D}[Z(x, y)]|^2$
- 3. Change PSD_{2D} map coordinates from Cartesian to Polar coordinates
- 4. Azimuthal average of PSD_{2D} to obtain $PSD_{surface}$.

The PSD_{scatter} from the scatterometer BRDF measurement is calculated using the Golden Rule (Eq 2.1).

4.1 Silicon wafer

Silicon wafers were one of the best polished, cleanest, most isotropic, highly reflective and cheapest surfaces available to us. A silicon wafer was subjected to profilometer (Figure 4.1) and scatterometer measurements for wavelengths ($\lambda_r = 633$ nm and $\lambda_b = 488$ nm) and 5° incidence angle. As shown in figure 4.2 below, surface and scatter measurements are consistent over the spatial frequency range not affected by the scatterometer signature ($f \ge 6$ cycles/mm). In other words, scatter introduced by surface roughness is correctly predicted by the profilometer measurement.

Similarly, the near specular scatter prediction of Rayleigh-Rice for the surfaces were verified. In order to shift the frequency corresponding to the instrument signature limitation to a frequency below $f_{\text{specification}}$ for ATST primary, the scatterometer must be used at very high angles of incidence - 84° for both 633 nm and 488 nm wavelengths. A comparison of the data (Figure 4.3) still shows satisfying agreement between the prediction from profilometer measurements and real scatter data at frequencies corresponding to near specular angles, for a smooth optical surface meeting the Rayleigh-Rice requirements.



Figure 4.1- Silicon wafer surface measured with the MFT 2.5x objective (RMS=1.44nm). Piston, Tip/Tilt, Power, Astigmatism, Coma and Spherical are removed to account for the MFT partial calibration for low frequencies.



Figure 4.2- Silicon wafer: PSD_{2D} from surface (MFT 2.5x objective) and scatter measurement ($\theta i = 5^{\circ}$, $\lambda_b = 488$ nm) comparison



Figure 4.3 Silicon wafer: PSD2D from surface (MFT 2.5x objective) and scatter measurement (θi = 84°, λ_b = 488 nm) comparison

4.2 Zerodur

Coated versus uncoated

A Zerodur optical flat ($\lambda/20$) was measured with the MFT before and after coating. The coating introduced pinholes (Figure 4.4a and 4.4b) changing the surface topography and making it slightly rougher. Consequently, the PSD of the surface has been modified.





Figure 4.4a - Uncoated Zerodur 1" optical flat RMS =2.1 nm measured with the MFT 2.5x objective over a 4.4x3.3 mm² FOV. Piston, Tip/Tilt, Power are removed. Surface height is in waves at 635 nm.

Figure 4.4b - 50 nm nickel coated Zerodur, 1" optical flat RMS =3.2 nm measured with the MFT 2.5x objective over a 4.4x3.3 mm² FOV. Piston, Tip/Tilt, Power are removed. Surface height is in waves.

A comparison of the $PSD_{surface}$ obtained from uncoated and coated Zerodur measurement shows that the nickel coated sample introduced a hump in its PSD from 5 cycles/mm where this was not the case for bare Zerodur surface (Figure 4.5). As expected the coated surface which was rougher has a PSD higher than for the uncoated area on mid-range frequencies.



Figure 4.5- Zerodur: PSD_{surface} for uncoated and coated surface measured with the MFT 2.5x objective over a 4.4x3.3 mm² FOV.

Scatter versus surface measurements

The PSD_{surface} of the coated surface was compared with PSD_{scatter} similarly to the Silicon wafer measurements. As five different spots were measured on the coated area of the Zerodur with the MFT, the PSD_{surface} considered was the averaged PSD adding the standard deviation (2σ) of those five measurements. In Figure 4.6 surface and scatter PSDs are plotted. The scatter PSDs presented on this graph were obtained at 5° incidence angle, using two different wavelengths $\lambda_r = 632.8$ nm and $\lambda_b = 488$ nm, on both sides of the specular beam. The PSD_{scatter} wavelength scales confirming, that after coating, the Zerodur surface still obeys the Rayleigh-Rice theory. As scatter data starts being believable from approximately f = 10 cycles/mm, it is noticeable that there is always at least one of the PSD_{scatter} curves passing through the PSD_{surface} error bars for f between 10 and 200 cycles/mm. That shows that a profilometric measurement properly predicts the scatter function introduced by surface microroughness for this sample. For frequencies smaller than 10 cycles/mm, the instrument signature of the scatterometer is prevalent over the scatter introduced by the surface topography. However, contrary to the silicon wafer's case, the coated Zerodur is contaminated by pinholes. Their contribution to direct scatter measurement at high angles of incidence (85°) is significant and overshadows the scatter introduced by surface topography. As such, in terms of PSD, scatter introduced by reflection on this surface looks about three orders of magnitude higher than what it would have been if scatter was only due to surface microroughness (Figure 4.7)- in other words, if all other sources of scatter contribution was negligible.



Figure 4.6- Coated Zerodur: PSD_{2D} from surface (MFT 2.5x objective) with 2σ error bars based on spots measured and scatter measurements ($\theta i= 5^{\circ}$, $\lambda_r = 632.8$ nm and $\lambda_b = 488$ nm) comparison.



Figure 4.7- Zerodur nickel coated: PSD_{2D} from surface (MFT 2.5x objective) and scatter measurement ($\theta_i = 5^\circ$, $\lambda_b = 488$ nm, $\theta_i = 5^\circ$, $\lambda_r = 632.8$ nm, $\theta_i = 85^\circ$, $\lambda_r = 632.8$ nm) comparison. At high angles of incidence, direct scatter measurements show a significant contribution of particle contamination to scattering (dark red curve): the PSD at small frequencies is about 3 orders of magnitude higher than expected.

5. CONCLUSION

This paper presents comparative results obtained from a scatterometer direct BRDF measurement and the BRDF prediction from a surface profile measurement for both a silicon wafer and a Zerodur optical flat ($\lambda/20$) coated with nickel. For surfaces meeting the Rayleigh-Rice requirements, this paper experimentally shows that a profilometric measurement of those surfaces allows, through their PSD calculation, accurate prediction of their BRDF over a wide range of directions, including angles very close to the specular direction, while those are usually inaccessible to scatterometers limited by their signature. Therefore, an easy profile measurement of optically smooth surfaces is a satisfying alternative to direct BRDF measurements. It has the advantage of predicting BRDF of almost any surface, regardless to the material, shape or direction to specify. This is of prime interest for measuring BRDF of optics such as the primary mirror of the ATST. However, for surfaces not meeting the Rayleigh-Rice requirements, a direct BRDF measurements remains the most reliable and straightforward approach.

As regards the particular example discussed in this paper of a scatter specification very near to specular, we have also illustrated a technique for increasing the angle of reflected scatter relative to specular. At a particular spatial frequency and wavelength, increasing the angle of incidence to near grazing will move the reflected scattered light farther from specular than is the case when using near normal incidence. This moves the scatter signal away from scatter due to the instrument, or away from the instrument signature, increasing the precision of the measurement

6. ACKNOWLEDGEMENTS

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