RMS Roughness, Total Integrated Scatter and Fractional Scatter of Production Parts

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Introduction

The limitations related to using total integrated scatter (TIS) to determining root mean square roughness (RMS) are reviewed and a new term, fractional scatter, is introduced that expands the roughness range over which scatter can be used to detect and monitor roughness changes in production surfaces.

Quantifying Roughness

Roughness is usually thought of as height variations in the surface profile; however, length variations are also important. Consider a sinusoidal surface of constant amplitude (height). If the sinusoidal wavelength is increased (decreasing the frequency) the surface may appear smoother. These length variations are usually expressed as spatial frequencies and they play an important role in quantifying roughness. A more complete presentation of the following material can be found in Chapter 2 of reference 1.

Assume we know a surface profile z(x) over some length L. Then the average surface height, will be $\bar{z}$ which is the average value of z(x) over L. The RMS roughness is then

$$\sigma = \left(\lim_{L \to \infty} \frac{1}{L} \int_{-L/2}^{L/2} [z(x) - \bar{z}]^2 \, dx \right)^{1/2} \quad . \tag{1}$$

Notice in the above equation that the value of roughness may change with the profile length L. In fact, common sense indicates that it is very likely to change. Higher frequency wiggles on a random surface generally tend to have lower height amplitudes. The larger the value of L is the more likely it is that the measured z(x) will have larger height maximums and thus a larger rms roughness. This reasoning leads to the insight that expressing roughness as a function of spatial frequency will be useful. This is easily done by taking the Fourier Transform, $Z(f_x, L)$, of the profile to reveal spatial frequency content. It has units of length squared.

$$Z(f_x, L) = \int_{-L/2}^{L/2} z(x) e^{-j2\pi f_x x} \, dx \tag{2}$$

After some manipulation (see Ref 1), the squared value of $Z(f_x, L)$ can be related to the roughness power (height squared) per unit spatial frequency. This function, called the power spectral density (or PSD) provides easy insight into the surface roughness characteristics. It has units of length cubed, which corresponds to height squared/unit spatial frequency.

$$PSD = S_1(f_x) = \lim_{L \to \infty} \frac{1}{L} |Z(f_x, L)|^2 \quad . \tag{3}$$

The absolute square in the above equation makes the PSD symmetrical. If z(x) is an expression then L can be infinite because all points on the profile will be known. So, the PSD can be found over the frequency range zero to infinity. In real profile measurement situations, the scan is limited to length L and the profile is sampled N times. Thus the minimum useful spatial frequency is limited to about 2/L, or two spatial wavelengths in the measured profile. The highest possible frequency is then limited by the Nyquist Theorem to N/2L, which corresponds to a wavelength of two sampling distances. The subscript 1 is used to indicate that the profile data came from a linear scan (rather than an area scan where a subscript 2 would be used and the Fourier Transform would be over both f_x and f_y for a z(x,y) profile). Figure 1 shows a hypothetical PSD of a surface with both random and periodic roughness.

In a real z(x) measurement situation there are usually dozens of parallel scans taken and the resulting PSD's are averaged to produce an "expected" PSD. This operation is usually performed automatically in the measurement instrument.

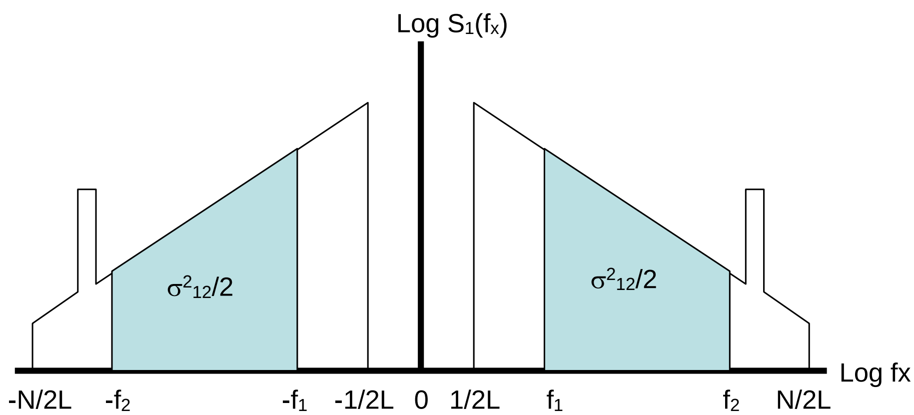

Figure 1. A hypothetical PSD is shown above on a log log plot. Symmetry and the max and min spatial frequencies are shown. The shaded areas from f1 to f2 and –f1 to –f2 illustrate that integration of the PSD gives the related bandwidth limited mean square roughness. Clearly calculated vales of σ depend on the associated bandwidth. The high frequency peaks represent the presence of a repetitive surface wave.

Figure 1 implies that the mean square roughness can be found by integrating the PSD over a band of frequencies. This makes it very clear that there is no such thing as one roughness value for a surface. Instead there is a rms value associated with a specific spatial bandwidth and thousands of those can be defined. Finally notice that changing the low frequency limit will have a much larger effect on σ than changing the high frequency limit where the PSD almost always has much smaller values. So if you are trying to compare measured roughness values from two different instruments, get at least the low frequency limits equal. All of this means that in general you should expect different rms roughness values when a sample is measured on different instruments – because they probably have different low frequency limits. In the real measurement world z(x) is not known – it is only sampled. This makes the calculation of the PSD and the rms roughness a little more complicated. See reference 1 for more details.

In a similar fashion we will see that integrated scatter changes with integration angle limits. The similarity is no accident.

Quantifying Light Scatter and Relating it to Roughness

Scatter signals can be easily quantified as scattered light power per unit solid angle (in watts per steradian); however, in order to make the results more meaningful, these signals are usually normalized, in some fashion, by the light incident on the scatter source. In this article we restrict the discussion to light scattered from just surface roughness and avoid the complexities associated with scatter from small discrete features such as pits and particles. We will further restrict the discussion to roughness profiles that do not change much over the area of the illuminated spot from which the scatter is coming. So, over the larger sample area the surface statistics (the PSD) may change, but can be considered constant within the illuminated spot.

For this situation it makes sense to normalize the scatter per unit solid angle by the incident power. This simple ratio, which has units of inverse steradians, was commonly referred to as “angle resolved scatter” or the ARS. This term is still found in the literature, but it has been generally replaced by a closely related function, the bi-directional reflectance distribution function (or BRDF), which is defined by forming the differential ratio of the sample radiance normalized by its irradiance. After some simplifying assumptions are made, this reduces to the original (ARS) scattering function with the cosine of the polar scattering angle in the denominator. The BRDF, defined in this manner, has become the standard way to report angle-resolved scatter from roughness and other features (oxide coatings, etc.) that uniformly fill the illuminated spot. We have NIST to thank for this basic definition and ASTM and SEMI to thank for written standards for the measurements. The cosine term results from the fact that NIST defined BRDF in radiometric terms.

$$\mathrm{BRDF} \equiv \frac{\mathrm{radiance}}{\mathrm{irradiance}} \cong \frac{P_s / \Omega_s}{P_i \cos\theta_s} \quad . \qquad (4)$$

The ARS is also sometimes referred to as the "cosine corrected BRDF" and is simply equal to the BRDF multiplied by the cosine of the polar scattering angle. Figure 2 gives the geometry for the situation, and defines the polar and azimuthal angles (θ_s and ϕ_s) as well as the solid collection angle (Ω). The BRDF has units of inverse steradians and is usually measured by moving a circular collection aperture in some path across the scattering hemisphere. Figure 2 also shows that transmissive scatter (BTDF) is defined in the same way. The term BSDF is used generically to include both reflective and transmissive scatter.

Care has to be taken that the data is representative of the sample, or of the situation being investigated, as the scatter patterns of non-uniform and/or non-isotropic surfaces can exhibit a lot of structure. An extreme case is scatter (diffraction) from a grating which will produce a series of bright peaks in the hemispherical pattern. Scatter from surfaces scratches and steps will exhibit a streak of light. In cases where the pattern is dominated by a streak of light, it often makes sense to take the measurement using a slit aperture (perpendicular to the streak) and normalize by the slit width (Δθ in degrees) instead of the aperture solid angular area in steradians. These cases are called "one dimensional" in nature because the surface frequencies associated with the feature "propagate" in only one direction. It is not reasonable to compare BRDF levels between one dimensional and two dimensional measurements. See Reference 1 for more details.

$$1D\,\mathrm{BRDF} \equiv \frac{\mathrm{P_s} / \Delta\theta_s}{\mathrm{P_i} \cos\theta_s} \; . \tag{5}$$

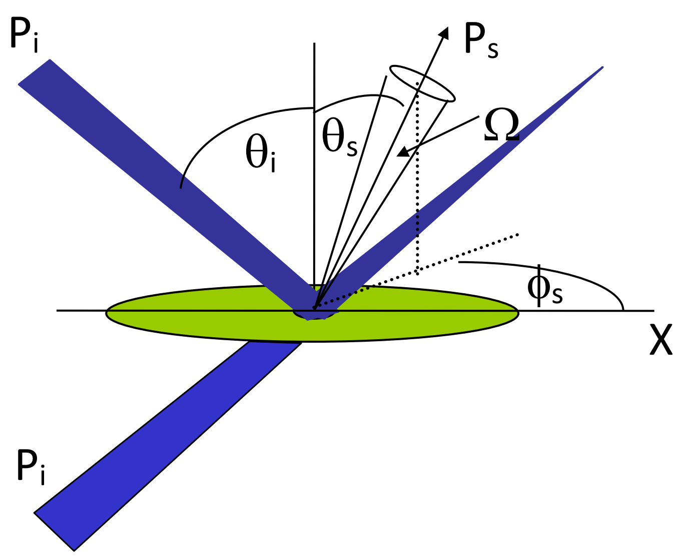

Figure 2. Standard spherical coordinates are used to define the geometry for the definitions of BRDF and BTDF.

Integration of the BRDF over much of the scattering hemisphere allows calculation of the "total integrated scatter," or TIS. This integration is usually carried out experimentally in such a way that the incident beam, the reflected specular beam and the integrated scatter are measured separately. In the most common TIS situation, the beam is incident on the sample at near normal and the integration is carried from small values of θ_s to almost 90 degrees over the hemisphere. If the fraction of light scattered from the specular reflection is small and if the scatter is caused by surface roughness, then it can be related to the rms surface roughness of the reflecting surface. In this case, it makes sense to normalize the scatter measurement, P_s, by the total reflected power, which is the specular reflection P_0 and P_s which is now the scatter integrated over most of the hemisphere. This is done because reductions in scatter caused by low reflectance should not influence the roughness calculation. As a ratio of powers, the TIS is a dimensionless quantity. The pertinent relationships are given below, where σ is the rms roughness and λ is the light wavelength.

$$\mathrm{TIS} \equiv \frac{P_s}{P_0 + P_s} = 1 - \exp[-(\frac{4\pi\sigma\cos\theta_i}{\lambda})^2] \cong \frac{P_s}{P_0} \cong \left(\frac{4\pi\sigma\cos\theta_i}{\lambda}\right)^2 . \qquad (6)$$

Of course, all scatter measurements are integrations over a detector collection aperture, but the TIS designation is reserved for situations where the attempt is to gather as much scattered light as possible, while "angle resolved" instruments are created to gain information from the distribution of the scattered light. Reference 1 discusses a number of subtleties associated with the TIS rms roughness relationship. One of which is a mistake made in the stray radiation code industry. Somehow in the early days of that industry they mis-defined (or re-defined) TIS as all of the scattered light normalized by the incident light – essentially the diffuse reflectance. A change in sample color (reflectance) would change this ratio without a corresponding change in roughness. Not good if the objective is rms roughness. Be careful what definition is being used when reading documents.

The TIS was defined by Bennett and Porteus in 1961 (ref 2) and the exponential relationship to roughness came from Davies in 1954 (ref 3) under the assumptions that the rms was much less than a wavelength and that the surface roughness had Gaussian statistics. The Gaussian assumption made the math easy for him, but a few decades later caused all kinds of trouble. The exponential expression turns out to be correct for any real optically smooth surface. When differences in calculated roughness were consistently observed between scatter measurements and profilometer measurements, the Gaussian assumption was blamed. If you are a careful reader you are already aware the problem was the difference in the lower bandwidth limit between the two instruments. It took years for this to be accepted.

The TIS scatter collection angles (near specular and high angle) are associated respectively with the low and high spatial frequencies of the measurement bandwidth. The relationships are given by the "grating equations" which are shown below:

$$f_x = \frac{\sin\theta_s \cos\varphi_s - \sin\theta_i}{\lambda} \quad , \tag{7}$$

$$f_y = \frac{\sin\theta_s \sin\varphi_s}{\lambda} \quad , \tag{8}$$

The frequency *f* associated with any direction in the hemisphere is equal to the square root of the quadrature sum of the x, y components as $f = (f_x^2 + f_y^2)^{1/2}$.

If the TIS, which can be found by integrating the ARS, gives the rms roughness, then it makes sense that the ARS (and the BRDF) should be related to the PSD as long as the scatter comes exclusively from roughness and the roughness is much less than a wavelength. The equation, called the Rayleigh-Rice relationship, brought into the optical scattering community by Gene Church (ref 4), is shown below:

$$\text{BRDF} = \frac{dP/d\Omega}{P_i \cos\theta_s} = \frac{16\pi^2}{\lambda^4} \cos\theta_i \cos\theta_s \, Q \, S(f_x, f_y) \ . \tag{11}$$

The angles are identified in Figure 2 and Q is the polarization factor. It is a real number less than 1.0, equals the Fresnel Reflectance in the specular direction, contains the sample index information and is detailed in ref 1. $S(f_x, f_y)$ is the two dimensional PSD. The relationship has been experimentally verified many times by changing the incident angle and/or the wavelength (thus changing the BRDF) but not changing the calculated PSD.

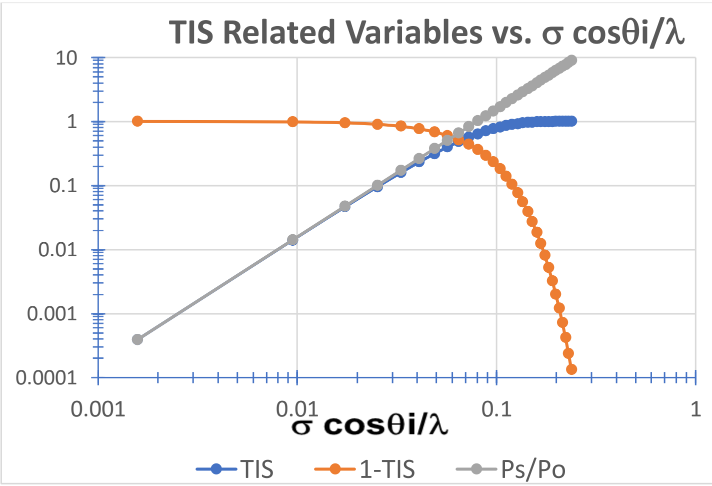

Figure 3. The TIS exponential and approximate form are plotted with (1-TIS) exponential form against ($\sigma \cos\theta_i/\lambda$) to indicate that the useful measurement range is no more than $\lambda/5$ for small incident angles.

Equations 8 and 11 are limited to “smooth optical surfaces.” When working in the visible you can check this by looking for your face in the sample. Another approximate check for optical smoothness is the Rayleigh criterion ($[4\pi\sigma \cos\theta_i/\lambda]^2 << 1$) which limits the size of the exponent in Equation 8. Neither “limit” is very exact, but the problem is put into perspective in Figure 3 where the exponential and approximate form (P_s/P_0) of the TIS are plotted against ($\sigma \cos\theta_i/\lambda$). For low incident angles the cosine is essentially one and the horizonal axis reaches a value of approaching 0.2 as the exponential form of the TIS saturates at 1.0. This tells us that the upper roughness limit where the exponential form of the TIS can be used to find roughness is at most a fifth of a wavelength. In other words, a TIS system (Figure 4) can be used to find the roughness of a polished silicon wafer (see Figure 5 below), but not the unpolished backside (see Figure 6). The approximate TIS value (P_s/P_0) will keep on increasing in value (above 1.0) as the surface roughens and will curve up at higher roughness levels as P_s increases and P_0 decreases. At higher roughness levels the measurement of P_0 becomes dependent on detector aperture size as well as roughness. Although the roughness value cannot be determined from P_s/P_0 for larger values, the ratio can be usefully used to track increasing roughness. For example, it might be useful to establish a signal level that indicates a backside is too rough to be held by either an electrostatic chuck or a vacuum chuck. Using P_s/P_0, instead of the diffuse reflectance (P_s/P_i), is better because it is independent of surface color changes. As long as the measurement stay consistent the result will indicate a change in roughness. One other point is worth mentioning. The approximate value of TIS reaches 1.0 at a value of σ/λ at less than 0.1. So, using the exponential form for the TIS over the approximate form in SEMI standards will more than double the roughness range that can be measured.

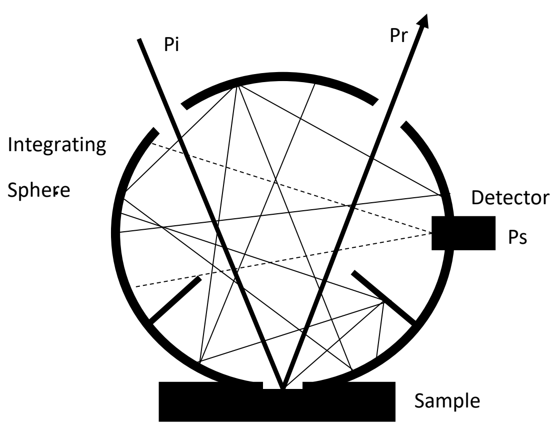

Figure 4. TIS measured in an integrating sphere system

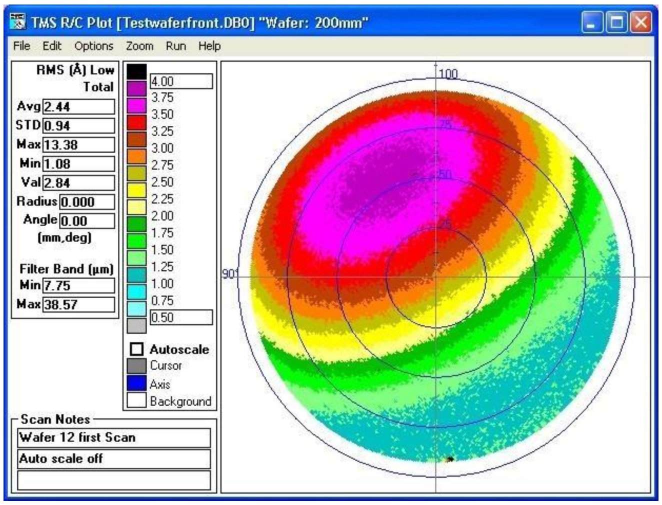

Figure 5. The color plot is a TIS measurement of rms roughness in Angstroms on the polished surface of a 200 mm wafer. Roughness variations of this sort are not uncommon. The data was taken on a TMS 2000W.

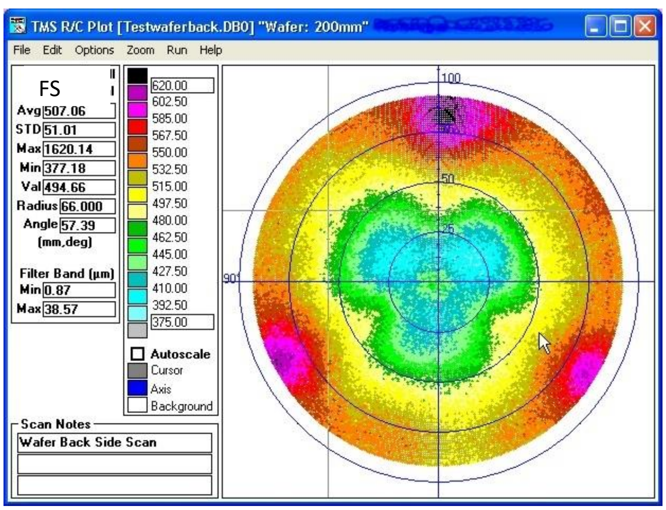

Figure 6. The Fractional Scatter is used to reveal changes in surface roughness on the backside of a wafer and an unexpected pattern is revealed.

The data in Figures 5 and 6 was taken with a TMS instrument manufactured by The Scatter Works, Inc. Basically TIS measurements are made on wafers (or other reflectors) in a programmable map over the sample and the results converted to surface roughness or other parameters such as fractional scatter, haze or diffuse reflectance.

References

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