Measurement and Effects of Surface Defects and Quality of Polish

Lionel R. Baker, Harold E. Bennett
Chairmen/Editors

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MEASUREMENT AND EFFECTS OF
SURFACE DEFECTS AND QUALITY OF POLISH

Volume 525

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MEASUREMENT AND EFFECTS OF SURFACE DEFECTS AND QUALITY OF POLISH

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INTRODUCTION

There have been two previous SPIE meetings concerned with the quality of optical surfaces. In 1979 the meeting was entitled "Contemporary Optical Systems and Components Specifications," (SPIE Vol. 181), and in 1982 the subject was "Scattering in Optical Materials," (SPIE Vol. 362).

Now, three years later, we return to report recent progress in this important, but somewhat neglected, field of optics. The subject has not attracted the importance it deserves, probably due to its negative overtones. No one actually wants surface defects or poor polish—they don't help you to do anything.

Whether or not people object to these defects, we know they are always likely to be present, and we have accepted that. Before we can define thresholds of acceptance and so write standards which will be used, we must first find generally agreed methods of measurement. Associated with these methods of measurement there must also, of course, be traceability back to national standards.

At a meeting held recently at Sira to report on and discuss the extent to which existing standards relating to surface quality were actually used by industry, it became clear that this subject was becoming of widespread interest and that most companies were calling for improved standards. The ophthalmic industry was worried about appearance defects, which had to be quantified in some way before thresholds of acceptance could be defined. The manufacturers of laser optics required the highest quality of surface finish because minute defects degraded performance. The same could be said of semiconductor-device manufacturers who deposited thin film structures with dimensions approaching those of the residual defects and debris left from even the best surface processing and finishing operations and from handling. The lifetime of high-performance-bearing surfaces depended on surface irregularities of micron dimensions.

In spite of the growing importance of surface defects in the optics, electronics, and mechanical engineering industries, there are still no generally accepted methods of measurement or standards defining thresholds of acceptance. The subject is not easy. It took decades to develop standards of surface finish using the contacting stylus. But we have the SPIE and easy means of communication between the various groups interested in this subject. It is up to us now to make the best use we can of the facilities they have provided.

This meeting was set up to bring together all the various interests, to report on recent developments including basic theory, practical measurement techniques, activity on standards, and to hear the comments and views of the manufacturers and users depending on us to provide methods of measurement and standards which they will find economic to use. Judging from present trends, it will not be long before industry will be seeking completely automatic methods of measuring surface quality. Perhaps that will be the subject of our next meeting in 1988—if not before!

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Session 1

Theoretical and Practical Aspects of Surface Defects

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Surface Roughness Metrology by Angular Distributions of Scattered Light

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Abstract

On-line industrial inspection of batch manufactured parts requires fast measurement techniques for surface finish quality. In order to develop the measurement basis for these techniques, a system has been built to determine surface roughness by measuring the angular distributions of scattered light. The system incorporates data gathered from the angular distribution instrument and traditional surface stylus instruments. These data are used both as input and as comparison data in order to test various mathematical models of optical scattering phenomena. The object is to develop a mathematical model that uses the angular distribution of scattered light to deduce surface roughness parameters such as R_a and surface wavelength. This paper describes the results of an experiment in which angular scattered data from surfaces with sinusoidal profiles was used to compute the surface R_a and wavelength. Stylus measurements of these parameters were made separately. A comparative table is given of the computed and measured values. Estimates of uncertainties are also given.

Introduction

On-line measurement of surface finish for metalwork manufacturing is a focus for our work in optical scattering at the National Bureau of Standards (NBS). Recent efforts by the manufacturing community to improve productivity through automation and greater quality assurance have emphasized the need for high speed, remote measurement techniques for monitoring surface finish. Typically these measurements would be performed at a time during manufacturing when, for example, a robot presents a part for inspection between processes, or during transfer from one machine to another, or at the time of an assembly operation.

This paper describes how our program at NBS provides the basis for relating area-based light scattering methods for measuring surface roughness to the more conventional stylus instrument. Results of our work are being used to aid the design of surface roughness measurement devices that will be installed in the Automated Manufacturing Research Facility (AMRF) at NBS. This facility is being developed at NBS in order to address the measurement and standards needs for the automation of small batch, discrete parts manufacturing industries [1]. Our optical measurement work began in a joint project with NASA for whom we are developing a prototype light scattering instrument to characterize the surface topography for model surfaces used in high Reynold's number wind tunnel testing of aircraft models [2]. With the assistance of the NBS Office of Non-Destructive Evaluation, we are also testing our current optical scattering system as a device for calibrating or characterizing standard reference surfaces.

This paper is structured into two main parts. In the first part we give an overview of the optical and stylus components of our system and show how mathematical models will be used to relate the data obtained from each component. In the second part, we describe a particular application of our system to the problem of deducing parameters that define sinusoidal surfaces from a knowledge of the angular distribution of light scattered from them.

Optical Scattering/Stylus System

System Design

When a collimated beam of laser light is reflected by a rough surface, the radiation is scattered into an angular distribution according to the laws of physical optics. The intensity and the pattern of the scattered radiation depend on the roughness heights, the spatial wavelengths, and the wavelength of the light. This is illustrated in Figure 1. In principle, the entire angular distribution of the scattered radiation contains a great deal of information about the surface topography. This is the basis for the design of our optical scattering system in which we combine a traditional stylus profiling instrument with an optical instrument called DALLAS (detector array for laser light angular scattering) [3] and interface them to a central minicomputer. We can test various scattering theories using both the light scattering data and the stylus data as input to check the validity of the predicted surface related parameters. Preliminary results have been previously presented [4].

Figure 2 gives a block diagram of the system. In the DALLAS device, a beam of He-Ne laser light illuminates the rough surface under examination. The scattered radiation is collected, digitized, and routed to a local microcomputer for initial viewing and/or sent to a central minicomputer for use in testing scattering models. The scattering data can be compared in detail to angular scattering distributions generated by optical scattering models that operate on surface topographic data measured by stylus instruments. Our facility has both commercial stylus instruments to generate surface profiles and a three-dimensional stylus machine to generate surface topographic maps [5].

Optical Detector Component

The principal apparatus in our system for measuring intensity distributions as a function of scattering angle from surfaces is shown in Figure 3 and consists of an illumination system and a detection system.

The illumination system consists of a 5 mW He-Ne laser with linear polarization, a quarter-wave plate to produce circular polarization, an automatic shutter, and a rotating assembly of two mirrors to direct the laser beam onto the specimen surface. The angle of incidence may be varied by a stepping motor which controls the angular position of the mirrors. The illuminated region of the specimen is a spot approximately 2 mm x 3 mm, depending on the angle of incidence. The detection system consists of an array of 87 detectors spaced 2° apart in a semicircular yoke (diameter = 164 mm) which is centered on the illumination spot on the specimen. The yoke can be rotated about one axis by a stepping motor so that the detectors can sample practically the entire hemisphere of radiation scattered from the surface.

Each detector consists of a lens, an optical fiber, and a PIN Si photodiode with an integral op-amp circuit. Each lens has a diameter of 4.4 mm and subtends an angle of $\sim 1.5^{\circ}$ in the yoke. It collects the radiation and focuses it onto the fiber which transmits the radiation to the photodiode. The output voltage signals from the op-amps are scanned by a 100-channel scanner, digitized, and stored in the desktop microcomputer. At present, a single angular scan of the 87 detectors takes about 10 s and yields intensity distributions which span over 5 orders of magnitude in intensity. The rms noise of the apparatus is approximately 50 μV, and the saturation voltage of the detectors is about 9 V. The nonlinearity of two typical detectors was measured by comparing their voltage outputs with that of a highly linear, standard Si detector. Over a dynamic range of 10^5 in input light intensity, the nonlinearity of the output voltage was less than 2% or 50 μV, whichever was greater. The relative linearity of the 87 detectors with light intensity (tracking) has also been checked. Over 3 1/2 orders of magnitude of light intensity, the output voltages tracked one another with a standard deviation of 2% or 2.5 times the rms noise, whichever was greater [6].

Surface Measurement Parameters

The scattering surfaces that are of concern to our work are referred to as engineering surfaces and are produced by a wide variety of manufacturing processes. Their structures may be highly varied and complex. A milled surface, for example, has a strong lay pattern, is highly regular and periodic, whereas a bead blasted surface is isotropic (i.e., roughness measurements along any direction yield similar results) and its structure is highly random. Most engineering surfaces, however, have a certain degree of anisotropy and a combination of both periodic and random features. To quantify the study of surface topography a number of statistical functions and parameters have been developed. These characterize the two basic aspects of topography: the heights of the asperities (amplitude) and the longitudinal spacings between the asperities (wavelength) [7].

In accordance with the ANSI B46 standard, we use the roughness average (R_a) parameter as the primary amplitude measure. It represents the average deviation of a surface profile about its mean line, defined as:

$$R_a = (1/L) \int_0^L |y(x)| dx, \qquad (1)$$

where x is the distance along the surface, y(x) defines the height of the surface profile about the mean line and L is the traversing length. R_a is the most widely used surface parameter in the world, partly because it is easy to calculate [8].

Because they can be produced by any of a number of processes, the regime of engineering surfaces is wide ranging. Typical values for R_a range from 0.1 µm to 10 µm and typical wavelengths may range from 5 µm to 800 µm. In general, surface structures with wavelengths greater than 800 µm are usually classified as waviness or errors of form rather than roughness.

Stylus Component

The standard method for surface topography measurement has been the stylus technique. Within the bounds that stylus displacements represent a convolution of the tip geometry and the surface microgeometry, the surface profile accurately represents the surface peaks and valleys rather than some average property of surface deviations. The output may be digitized and analyzed in a computer to yield a variety of statistical parameters and functions for characterizing the surface with confidence that these closely represent true profile parameters. Fine resolution and wide range are also important features of stylus instruments. The ultimate vertical resolution is on the order of 0.3 nm rms and the range can be as much as 100 µm rms. The horizontal resolution is limited by the stylus width; it is typically several micrometers but can be as small as 0.1 µm, more than acceptable for most topographic measurements. For our measurements, the sample length of the profile is approximately 1.84 mm, and the point spacing is 0.46 µm. The horizontal resolution of the instrument is approximately 1 µm, limited by the high frequency falloff of the stylus response function. Each surface, in general, is sampled with up to 10 stylus traces evenly distributed over the surface area. Hence, the total amount of topography information amounts to about 40,000 digitized points for each surface. For a discussion of the uncertainties involved in stylus measurements see [9].

Mathematical Modeling Component

The electromagnetic properties of light provide us with a viable route to connect the angular distributions of light with the scattering surface. From Maxwell's equations the problem of finding the rectangular component of the scattered electric field for the direct light scattering problem reduces to solving

$$\nabla^2 E + k^2 E = 0 \quad (2)$$

at an observation point P (x_o, y_o, z_o) outside of a volume V bounded by the illuminated surface S. If R is the distance from a point (x, y, z(x,y)) on the surface S to P, then under the condition that the scattered electromagnetic field lies in the plane of incidence, the scalar component of the field at P is shown in [10] to be

$$E(x_o, y_o, z_o) = \left(\frac{1}{4\pi}\right) \iint_S \left(E \frac{\partial}{\partial n} (\mathrm{Exp}(i2\pi R/\lambda)/R) - (\mathrm{Exp}(i2\pi R/\lambda) \frac{\partial E}{\partial n}\right) ds , \quad (3)$$

where $\partial E/\partial n$ is the normal derivative at a point on S. This integral forms the basis of our present calculations and is called the Helmholtz integral. It involves the unknowns E, $\partial E/\partial n$ on the scattering surface S. Various particular models determine how E, $\partial E/\partial n$ are computed. For example, by using single or double layer potentials [11], one is led to an integral equation in order to compute E or $\partial E/\partial n$ on the boundary S. Another approach, the tangent plane or Kirchhoff method, relates E and $\partial E/\partial n$ on the surface directly to the known incident field. This is an approximation used to circumvent solving the integral equation for the boundary current. As a result, though, the Kirchhoff method is only applicable in certain regimes.

The optical scattering/stylus system gives us the framework to generate scattering data as well as surface characterization data in order to test specific model formulations for the surfaces of interest. Individual model performance can be measured by statistical confidence techniques. In particular, once a specific solution procedure is selected, the surface S is parameterized in some form by parameters p_j, j = 1,...,k. A sum-of-squares difference can be written as

$$H(p_1, \ldots, p_k) = \sum_J [\mathrm{DATA}(J) - \mathrm{SCI}(J, p_1, \ldots, p_k)]^2$$

where DATA(J) represents measured intensity values at a point indexed by J and $\mathrm{SCI}(J, p_1, \ldots, p_k)$ represents values at a point computed from (3), where the model intensities are defined by

$$J(x_o, y_o, z_o) = |E(x_o, y_o, z_o)|^2 ,$$

and are functions of the parameters p_j, $j = 1,\ldots,k$. $H(p_1,\ldots,p_k)$ is used to measure the goodness of fit of the computed scattered field to the experimentally determined field. A best-fit set of parameters will be that set which minimizes the sum-of-squares $H(p_1,\ldots,p_k)$.

After the sum is minimized, one can estimate approximate confidence regions for the individual parameters as follows. Let $p_o = (p_{o1},\ldots,p_{ok})$ be the vector of parameters that minimizes H. Suppose that there are n data values. Let

$$H_o = (H(p_o)/(n-k))^{1/2} \tag{4}$$

and let

$$c_j = 1/[\partial^2 H(p_o)/\partial p_j^2] \tag{5}$$

for $j = 1,\ldots,k$. A one parameter confidence interval about p_{oj}, $j = 1,\ldots,k$ can be constructed as

$$|p_{oj} - p_j| < [t_q(n-k)] (c_j)^{1/2} H_o \tag{6}$$

where $t_q(n-k)$ is the two-tailed q percentile point of the Student's t distribution. q can also be thought of as the confidence probability. For a discussion of the statistical assumptions involved see [12]. These confidence intervals are sets of the individual parameters for which one can assert that, given many repetitions of the experiment, the values of the separate parameters that minimize the sum-of-squares function will lie within those intervals with the prespecified probability q. They yield information on model response and do not take into account systematic or experimental uncertainties.

An Application to Sinusoidal Specimens

The stylus/optical scattering/computer system has the capability to test specific models for the scattering process as well as specific topographic models. We now describe a specific scattering model and the results of the parameter fitting. In order to separate the influence of scattering model errors and surface model errors in theoretical predictions of scattering distributions (intensities), we used sinusoidal surfaces as scattering specimens. These could be analytically defined and thus allowed us to isolate the fitting errors to the scattering model. Finally, we will give an example of the simple optimization methods we used to reconstruct the surface profile and return measures of profile R_a and wavelength.

Specific Mathematical Model

The first optical model tested is the general Kirchhoff approximation for the boundary values for E and $\partial E/\partial n$. In particular, we assume that incident field $\mathbf{E}_i$ is a harmonic plane wave of unit amplitude, having a propagation vector $\mathbf{K}_i$ with the magnitude, $K_i = 2\pi/\lambda$. On the boundary S we assume the following approximations: 1) The magnitude of the field E on S, E, equals $(1+\rho)$ times the magnitude of $\mathbf{E}_i$, and 2) $\partial E/\partial n$ on S is $(1-\rho)$ times the magnitude of $\mathbf{E}_i$ multiplied by the projection of the propagation vector $\mathbf{K}_i$ onto the normal to the surface S. ρ is the reflection coefficient of a smooth plane. It depends on the angle of incidence, the electrical properties of S and the polarization of the incident wave. Our next assumptions are that we have a perfectly conducting surface. In our case $\rho = 1$ (see [7]). Furthermore, we assume that the surface S is a function of one variable z(x), and that the illumination length $L >> \lambda$.

The geometry of the scattering problem (shown in Figure 4) is two dimensional. To a good approximation, the test surfaces may be assumed to be rough only in the x direction and smooth in the y direction. The plane of incidence of the light is the x,z plane. The incoming plane wave vector $\mathbf{K}_i$ has angle of incidence θ_i with respect to the normal vector n of the mean value plane of the surface. The functional form for the incident electric field $\mathbf{E}_i$ is given by $\exp(j\mathbf{K}_i\cdot\mathbf{r})$. The scattered electric field is to be evaluated for an angle θ_s with corresponding outgoing vector $\mathbf{K}_s$. The vector r extends from some nearby origin O to a point on the surface.

With the foregoing considerations and assumptions, the scattered electric field E can be calculated from equation (3) as a function of scattering angle θ_s in the Fraunhofer zone of the scattered field. It is given by the phase integral over the surface profile z(x):

$$E(\theta_s) = C_o (1+\cos(\theta_i - \theta_s))/(\cos(\theta_i)+\cos(\theta_s)) \int_0^L \exp(j\mathbf{V}\cdot\mathbf{r})dx \quad (7)$$

where $\mathbf{V} = \mathbf{K}_i - \mathbf{K}_s$, L is the length of the illuminated region along the x direction, and $\mathbf{r} = x\mathbf{i} + z(x)\mathbf{k}$. The vectors $\mathbf{i}$ and $\mathbf{k}$ are unit vectors in the x and z directions, respectively, $\mathbf{r}$ contains all of the information concerning the surface profile, and in detail,

$$\mathbf{V}\cdot\mathbf{r} = V_x x + V_z z$$

$$= 2\pi/\lambda[(\sin\theta_i + \sin\theta_s)x + (\cos\theta_i + \cos\theta_s)z(x)] \quad (8)$$

The sign convention here is such that $\theta_s = -\theta_i$ in the specular direction. C_o is a quantity which depends on a number of factors such as θ_i and $\mathbf{E}_i$, but is independent of θ_s. For the details of the derivation see [13].

Sinusoidal Surfaces

NBS is in the process of calibrating a set of precision roughness specimens [11], one series of which is available to the public through the Office of Standard Reference Materials [15]. These specimens were designed primarily to provide a means for optimum transfer of an accurate roughness average R_a value from primary to secondary laboratories. However, properties of the specimens also make them very useful for evaluating instrumentation and computational algorithms designed to measure the statistical parameters and functions now being investigated in many laboratories. Prototype specimens with an R_a value of 1.0 µm and wavelengths of 40, 100, 800 µm have been fabricated (Figure 5). Prototype specimens have also been fabricated for a wavelength of 100 µm and R_a values of 3.0 and 0.3 µm (Figure 6).

These specimens were designed: 1) To make specimen R_a insensitive to stylus radius, 2) to provide a good standard for surface statistical functions, and 3) to provide a good waveform for evaluating surface measurement instrument characteristics. Finally, they are also good test specimens for light scattering, which was the motivation for their selection as specimens for the work reported in this paper.

The surfaces were manufactured by means of diamond turning on a numerically controlled lathe. They were mounted around the periphery of a plate that was then placed in the lathe chuck. The tool tip was programmed to generate a sine wave in one dimension as it performed a linear translation in the other (Figure 7). Figure 8 plots the spectral density functions for the 1 µm R_a samples with 40, 100, 800 µm wavelengths. It illustrates the quality of the waves manufactured.

The particular R_a's and wavelengths for the surfaces were selected in order to provide samples that exhibited characteristics similar to manufactured surfaces. This is illustrated in Figure 9. Specimens with varying wavelengths were made from brass; those of different roughness amplitude were made from electroless nickel.

Optical Scanning Technique

For all our calculations the angle of incidence was chosen as $\theta_i = 45^\circ$. The laser used was He-Ne with $\lambda = 0.6328$ µm.

The angular distribution data acquired for the prototype SRM's was based on a special configuration of the DALLAS optical scattering device. In order to gain the resolution in the scattered data only one sensor at the top of the yoke was used. The laser beam was aimed in such a way that the plane of scattering was orthogonal to the axis of the yoke. The single sensor sampled the scattering from -90° to 0° where the sign convention indicates the specular direction quadrant. The backscatter quadrant was not sampled. The -90° represented the yoke in a horizontal position with the sensor furthest from the laser but in the plane of scattering. The 0° position represented the sensor in the vertical position. Sensor data values were taken in increments of 0.18°. This resulted in 501 angular distribution data points for the quadrant in the specular direction for each SRM prototype.

The optical sensor used was apertured to 1 mm. With a radial distance from the scattering surface of 164mm, the sensor subtended an arc of 0.35°. Numerically, a grid of scattering angles θ_s of sufficient fineness was used with equation (7) so that 47 intensity values were generated by the model within the angle subtended by the detector at one sampling position. These values were then averaged to simulate a sensor data value. The numerical scattering angle mesh width was 0.0075°.

Numerical Considerations

Since the surfaces we used were periodic, it is possible to simplify the scattering integral equation (7). Let z(x) be the surface profile and suppose that z(x) = z(x+D). Beckmann and Spizzichino [10] show that (7) can be reduced to

$$E(\theta_s) = W \sec\theta_i (1+\cos(\theta_i - \theta_s))/(\cos\theta_i + \cos\theta_s) (1/D) \int_0^D \exp(j\mathbf{V}\cdot\mathbf{r})dx \tag{9}$$

where $\mathbf{V}\cdot\mathbf{r}$ is given by (8),

$$W = (\sin 2np\pi / 2n\sin p\pi)\exp(-jp\pi) \tag{10}$$

and

$$p = (D/\lambda)(\sin\theta_i + \sin\theta_s). \tag{11}$$

We next assumed the profile function form z(x) = Asin(2πfx) as an adequate surface model, where A represented the amplitude in micrometers and f represented the spatial frequency in μm^{-1}. This function was introduced into the integral (9). For each A,f, Eq. (9) was evaluated over one wavelength with a mesh width of 1/100 of a wavelength. Simpson's quadrature rule was used for the integral. An 11 x 11 grid in (A,f) space was searched near the nominal surface parameter values for A and f for values that minimized the sum

$$H(A,f) = \sum_J [DATA(J) - SCI(J,A,f)]^2 . \tag{12}$$

The model values SCI(J,A,f) represented scaled values of the squared magnitude of $E(\theta_s)$ in (9). As an example of the result, Figure 10 shows the optical scattering pattern from the brass prototype sinusoidal surface with a nominal 1 μm R_a and surface wavelength of 100 μm. The nominal surface amplitude can be estimated as $A = \pi/2\ R_a$ which in this case is 1.57 μm. The nominal surface frequency f would be .01 μm^{-1}. Instead of using the entire 501 points we used 167 points of data covering approximately the middle 30° in the specular direction. This was done in order to restrict the calculation to the most significant region in the figure. A grid area from A = 1.55 to 1.75 μm in steps of 0.02 μm and f = 0.005 to 0.015 μm^{-1} in steps of 0.001 μm^{-1} was searched and the sum-of-squares difference (12) computed. The response surface was plotted in Figure 11 in a reciprocal form. The minimum sum is reflected as a maximum point. The grid minimum occurred at A = 1.59 μm and f = 0.01 μm^{-1}. In order to be more precise we performed a linear search along the ridge with f = 0.01 μm^{-1} fixed. This linear search is plotted in Figure 12. The minimum was found at 1.588 μm. The superposition of the 167 angular distribution data points and predicted intensities is plotted in Figure 13.

These steps were performed for five of the six prototype surfaces. The spatial grid chosen for numerical integration proved to be too coarse for the long 800 μm wavelength specimen. The comparisons are given in the next section. The technique of minimizing the intensity difference errors has been used previously by Aas [16]. His approach, though, was not to assume an analytic form for the surface profile but to adjust the points of a piecewise linear approximation to the surface profile, using a Newton minimization algorithm. In our case, a grid search was used since Newton algorithms are local minimization procedures, and we did not know what the response surface would look like in terms of the distribution of local minima.

Results

We summarize the measured and computed values for the roughness average (R_a) and the surface wavelength (D) in Table 1 (after the references). This table also includes three standard deviation estimates of confidence (3SD) for the numbers. Note that the confidence intervals for the measured values represent the combination of random and systematic uncertainties which have been developed after several years experience with the stylus instruments. The confidence intervals on the computed values represent random uncertainties due only to the mathematical fitting process. They are an indication of the structure of the sum-of-squares response surfaces near the optimum parameter values (e.g., Figure 11). The smaller the value the sharper the valley and the larger the value, the broader the valley at the minimum. R_a is computed from the amplitude by $R_a = (2/\pi)A$.

The R_a measured values in Table 1 are somewhat larger than previously published values [17]. While these are within the uncertainty bounds, the difference is probably due to the use in this work of a smaller radius stylus tip which reveals finer and additional texture in surface waveforms. The measured R_a's were based on roughness profiles of 4000 points.

Our results suggest that the Beckmann-Spizzichino form of the Kirchhoff model is sufficiently valid to be useful for estimating the roughness parameters of surfaces with roughness height on the same order as the optical wavelength and the surface wavelength much greater than it. In the future, we plan to extend the calculations from periodic to random surfaces in this general roughness regime.

Discussion: Model Validity

Wirgin [18] has discussed the validity of the Kirchhoff approximation for sinusoidal surfaces. Figure 14 shows a graphical picture of an extended region of validity given by Teague, et al. [19]. Let A represent one-half of the surface peak-to-valley (i.e., H = 2A), D the surface wavelength and the incident light wavelength. These studies of the validity regions relate the predictability of the optical scattering in terms of ratios of the three quantities A, D, and λ.

When the surface wavelength was approximately 10 times the wavelength of the incident light, Wirgin found that as the angle of incidence increased the amplitude of the surface had to decrease as a fraction of the surface wavelength. In particular, the Kirchhoff approximation was found to be sufficiently accurate at normal incidence for $A/D < 0.011 D/\lambda$. With increasing angle of incidence errors occurred for $A/D \geq 0.1$ above $\theta_i = 6^\circ$, for $A/D \geq 0.05$ above $\theta_i = 37^\circ$ and for $A/D \geq 0.016$ above $\theta_i = 63^\circ$. All of these cases assumed $D/\lambda = 10$.

For longer surface wavelengths, Wirgin found that surface amplitudes could be slightly larger. When D/λ was varied, significant errors occurred for D = 36, $A/D \geq 0.1$ only above $\theta_i = 25.5^\circ$. When $A/D \geq 0.13$, Wirgin found that the Kirchhoff approximation failed in general. Finally, his results indicate that no known theory predicts scattering well for $A/D \geq 0.16$ and $D/\lambda > 10$.

The table below lists surface ratios for the NBS prototype SRM's. In Table 2, R_a, D, A, and H are units of µm. Since $D/\lambda > 10$ for all our cases and $A/D < 0.16$, Wirgin's regions cannot be used directly to determine whether the Kirchhoff model would be appropriate in the SRM case. However, for $D/\lambda = 10$, Wirgin's data suggests that the Kirchhoff approximation would fail for $\theta_i = 45^\circ$ and $A/D \geq 0.04$. This would imply that in our case the 3.0 µm R_a surface might be on the borderline of the approximation. The point representing the 3.0 µm R_a surface is also outside of the estimated region of validity in Figure 10. Note that $A = \pi/2\ R_a$ was used to estimate the nominal A value.

Table 2

Surface Ratios for NBS Prototype SRM's

$\lambda = 0.6328$ µm

R_a	D	A	H	A/D	H/D	D/λ	λ/D
1	40	1.57	3.14	.039	.078	63.21	.016
1	100	1.57	3.14	.016	.032	158.03	.0063
1	800	1.57	3.14	.002	.004	1264.22	.000079
3.0	100	4.71	9.42	.047	.094	158.03	.0063
0.3	100	0.47	0.94	.0047	.0094	158.03	.0063

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Table 1

Measured and Computed R_a and D Parameters [2]

Surface	Nominal		Measured				Computed			
Type	R_a	D	R_a	3SD[1]	D	3SD	R_a	3SD	D	3SD
Brass	1	40	1.02	0.04	40.2	0.8	1.013	0.004	40.00	0.01
Brass	1	100	1.02	0.05	100	1	1.013	0.006	100	1
Brass	1	800	Measurements and Computations Still in Progress[3]							
Nickel	1	100	1.03	0.05	100.0	1.2	1.011	0.005	100	1
Nickel	0.3	100	0.31	0.03	100.1	1.5	0.311	0.009	100.0	1.6
Nickel	3	100	2.98	0.07	100	1	3.008	0.016	100	3

(1) 3SD stands for a three standard deviation estimate.

(2) All numbers are in units of μm.

(3) The nature of the fitting process for the long wavelength surfaces is somewhat different.