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Random Process Model of Rough Surfaces[1]

Rough surfaces are modeled as two-dimensional, isotropic, Gaussian random processes, and analyzed with the techniques of random process theory. Such surface statistics as the distribution of summit heights, the density of summits, the mean surface gradient, and the mean curvature of summits are related to the power spectral density of a profile of the surface. A detailed comparison is made of the statistics of the surface and those of the profile, and serious differences are found in the distributions of heights of maxima and in the mean gradients. Techniques for analyzing profiles of random surfaces to obtain the parameters necessary for the analysis of the surface are discussed. Extensions of the theory to nonisotropic Gaussian surfaces are indicated.

1 Introduction

The characterization of the topography of solid surfaces is of interest in the study of a number of interfacial phenomena such as friction and wear, and electrical and thermal contact resistance.

A very general typology of solid surfaces is shown in Fig. 1. Surfaces that are deterministic may be studied by relatively simple analytical and empirical methods; their detailed characterization is straightforward. However, many engineering surfaces are random; and it is these that have been subjected to a great deal of study in the past decade.

In this paper, attention is concentrated on random, isotropic, Gaussian surfaces, although extensions of the theory to nonisotropic surfaces are indicated. It is clear [1][2] that many surfaces are non-Gaussian; but it is equally clear that many surfaces are Gaussian [1]. Moreover, a study of Gaussian surfaces should provide a good preparatory background for the study of non-Gaussian surfaces.

Our approach is to use the techniques of random process theory. The height of a rough surface may be considered to be a two-dimensional random variable, with the Cartesian coordinates in a reference surface being the independent variables. This approach was first used by Longuet-Higgins in 1957 in two outstanding studies of random ocean surfaces [2, 3]. Some of the results reported in the following sections are from Longuet-Higgins' work, and, in these instances, we shall refer the reader to his work for proofs of statements.

A brief survey of the literature on surface mechanics has revealed a number of attempts to analyze solid surfaces with the techniques of random processes [4–6]. All these analyses, however, rest on two assumptions, both of which are shown to be unnecessary in the present work: (1) The statistics of the surface are the same as the statistics of a profile of the surface, and (2) the asperities have spherical caps. The first assumption is found in the following pages to lead to serious error. It is necessary to distinguish a peak on a profile from a summit on the surface, to use the terminology of Williamson and Hunt [7]. A profile will more often than not pass over the shoulder of an asperity on the surface instead of its summit. The shoulder will, nevertheless, appear as a peak on the profile, though one of reduced height. Thus the profile indicates the presence of far fewer high peaks than actually exist on the surface. A similar error occurs in the determination of the mean surface gradient; it is not the same as the mean slope on a profile. Both of the foregoing assumptions are dropped in the present work.

In Section 2, some of the relevant results of random process theory are summarized. Further details may be found in the work of Longuet-Higgins [2, 3]. In Section 3, various results are obtained for random, isotropic, Gaussian surfaces. In Section 4, the sampling of such surfaces by profilometry is

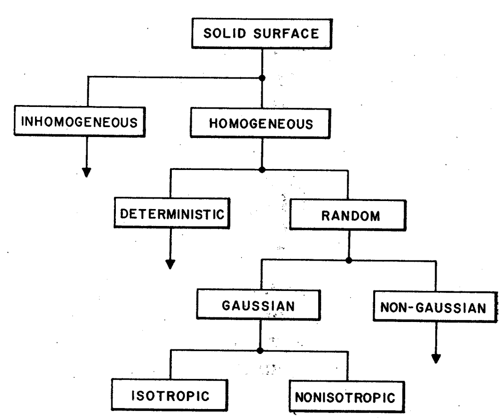

Fig. 1 A general typology of surfaces

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[2] Numbers in brackets designate References at end of paper.

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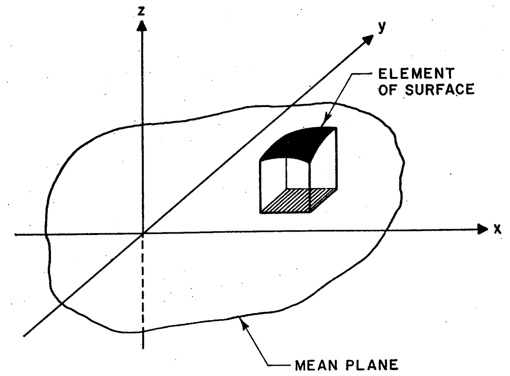

Fig. 2 Rough surface coordinates

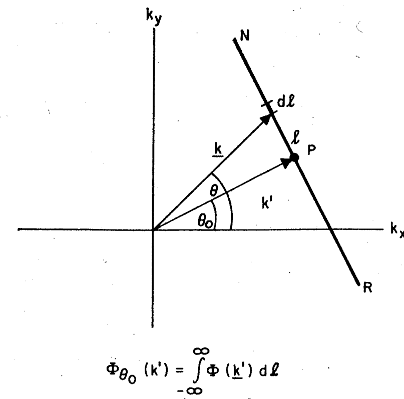

Fig. 3 Generation of the PSD of the θ_0 profile from the PSD of the surface

analyzed. Results are given for the statistics of profiles, and a comparison is made of surface and profile statistics. In addition, a very simple technique is described for obtaining all the parameters necessary for the analysis of Section 3. Some conclusions are presented in Section 6, together with indications of extensions of the theory to nonisotropic Gaussian surfaces.

2 The Characterization of Random Processes [2]

The Autocorrelation Function. Consider a rough surface whose height above a plane reference surface is $z(x, y)$, where z is a random variable and x, y are Cartesian coordinates in the reference surface, Fig. 2. The reference surface may be taken to be the mean plane of the rough surface. We assume that the surface is homogeneous—that is, its statistical description is invariant with respect to translation along the surface. The autocorrelation function is then defined to be

$$R(x, y) = \lim_{\substack{L_1 \to \infty \\ L_2 \to \infty}} \frac{1}{4L_1L_2} \int_{-L_1}^{L_1} \int_{-L_2}^{L_2} z(x_1, y_1) \times z(x_1 + x, y_1 + y) dx_1 dy_1. \quad (1)$$

If the surface is isotropic, R depends only on $r = (x^2 + y^2)^{1/2}$, and not on the polar angle $\theta = \tan^{-1}(y/x)$.

The Power Spectral Density (PSD). The Fourier transform of R is called the power spectral density:

$$\Phi(k_x, k_y) = \frac{1}{4\pi^2} \iint_{-\infty}^{\infty} R(x, y) \exp\,[-i(xk_x + yk_y)] dxdy. \quad (2)$$

The inverse Fourier relation holds:

$$R(x, y) = \iint_{-\infty}^{\infty} \Phi(k_x, k_y) \exp\,[i(xk_x + yk_y)] dk_x dk_y. \quad (3)$$

k_x and k_y are the components of a wave-vector $\mathbf{k}$. From equation (1), we see that $R(0, 0)$ is σ^2, where σ is the rms roughness, or the standard deviation of the roughness. It then follows from equation (3) that

$$\sigma^2 = \iint_{-\infty}^{\infty} \Phi(k_x, k_y) dk_x dk_y. \quad (4)$$

Equation (4) indicates that $\Phi(k_x, k_y)$ is a decomposition of σ^2 (the power in electrical terminology, when the random variable is a current) into contributions from various spectral components, which are waves with wave-number $\mathbf{k}$. The wavelength of these waves is

$$\lambda = 2\pi/|\mathbf{k}|, \quad (5)$$

and their direction is along

$$\theta = \tan^{-1}(k_y/k_x). \quad (6)$$

For isotropic surfaces, Φ depends only on $k \equiv |\mathbf{k}|$.

The Autocorrelation and PSD for a Surface Profile. If a profile of the surface be taken in the plane $\theta = \theta_0$, the height z of the profile is a function only of the distance r from the origin along the profile. The autocorrelation and the PSD for the profile are defined to be

$$R_{\theta_0}(r) = \lim_{L \to \infty} \frac{1}{2L} \int_{-L}^{L} z(r_1) z(r_1 + r) dr_1, \quad (7)$$

and

$$\Phi_{\theta_0}(k') = \frac{1}{2\pi} \int_{-\infty}^{\infty} R_{\theta_0}(r) \exp\,(-ik'r) dr. \quad (8)$$

Relation Between Surface and Profile PSD's. Longuet-Higgins [2] shows that the following relation holds between Φ and Φ_{θ_0}:

$$\Phi_{\theta_0}(k') = \int_{-\infty}^{\infty} \Phi(k_x, k_y) dl, \quad (9)$$

where

$$l = (k_x^2 + k_y^2 - k'^2)^{1/2}. \quad (10)$$

The physical meaning of equation (9) may be clarified with the help of Fig. 3. The point P in the wave-number plane has coordinates ($k' \sin \theta_0$, $k' \cos \theta_0$). It represents waves with wave-number k' along the profile. The line NPR, perpendicular to $0P$, is the locus of all wave numbers whose projection on $0P$ is k'. Thus, any wave with a wave vector lying on NPR appears to have a wave-number k' in a section parallel to $0P$. The line NPR is the path of integration in equation (9).

Moments of the PSD. The moments m_{pq} of Φ are defined as follows:

$$m_{pq} = \iint_{-\infty}^{\infty} \Phi(k_x, k_y) k_x^p k_y^q dk_x dk_y. \quad (11)$$

It follows from equation (4) that

$$m_{00} = \sigma^2. \quad (12)$$

The moment $m_{n\theta_0}$ of the profile is defined as follows:

$$m_{n\theta_0} = \int_{-\infty}^{\infty} \Phi_{\theta_0}(k')(k')^n dk'. \quad (13)$$

The following relation exists between the m_{pq} and the $m_{n\theta_0}$ [2]:

$$m_{n\theta_0} = m_{n0} \cos^n\theta_0 + C_1^n m_{n-1,1} \cos^{n-1}\theta_0 \sin\theta_0 + C_2^n m_{n-2,2} \cos^{n-2}\theta_0 \sin^2\theta_0 + \ldots + m_{0n} \sin^n \theta_0, \quad (14)$$

where

$$C_m^n = n!/m!(n - m)!. \quad (15)$$

Equation (14) may be derived by combining equations (9), (11), and (13). When the surface is isotropic, the following relations may be derived from equations (11) and (14):

$$\left.\begin{aligned} m_{20} = m_{02} = m_2; \quad m_{11} = m_{13} = m_{31} = 0; \\ m_{00} = m_0; \quad 3m_{22} = m_{40} = m_{04} = m_4. \end{aligned}\right\} \quad (16)$$

In equation (16), the subscript θ_0 for the moments of the profile PSD is dropped, since isotropy implies that the profile statistics are independent of the direction θ_0 of the profile.

The Central Limit Theorem. Let $\xi_1 \ldots \xi_n$ be n quantities, each of which is the sum of a large number of independent variables with zero expectation. Then, under very general conditions [8], the joint probability density of the ξ_i is Gaussian in n dimensions:

$$p(\xi_1 \ldots \xi_n) = (2\pi)^{-\frac{n}{2}} \Delta^{-1/2} \exp\,\{-\tfrac{1}{2} M_{ij}\xi_i\xi_j\}, \quad (17)$$

where the matrix M is given by

$$M = (N)^{-1} \quad (18)$$

and

$$N = \begin{pmatrix} \overline{\xi_1^2} & \overline{\xi_1\xi_2} & \ldots & \overline{\xi_1\xi_n} \\ \overline{\xi_2\xi_1} & & & \\ \overline{\xi_n\xi_1} & \ldots & \ldots & \overline{\xi_n^2} \end{pmatrix}, \quad (19)$$

and

$$\Delta = \text{Det.}(N_{ij}). \quad (20)$$

The element $\overline{\xi_i\xi_j}$ of the matrix is defined by

$$\overline{\xi_i\xi_j} = \int \ldots \iint_E \xi_i(\epsilon_1 \ldots \epsilon_k)\xi_j(\epsilon_1 \ldots \epsilon_k) p(\epsilon_1) \ldots p(\epsilon_k) d\epsilon_1 \ldots d\epsilon_k, \quad (21)$$

where E is the probability space of the independent random variables ϵ_j on which the ξ_i depend.

3 The Statistics of Random, Isotropic, Gaussian Surfaces

Assume that the surface height $z(x, y)$ may be represented by the infinite sum

$$z(x, y) = \sum_n C_n \cos\,(xk_{xn} + yk_{yn} + \epsilon_n). \quad (22)$$

It is assumed in equation (22) that there are an infinite number of wave-vectors (k_{xn}, k_{yn}) in any area $dk_x dk_y$. ϵ_n is a random phase, with a uniform probability of lying in the range $(0, 2\pi)$. The coefficients C_n are related to the PSD Φ by

$$\Phi(k_x, k_y) dk_x dk_y = {}^1/_2 \sum_{\Delta k} C_n^2, \quad (23)$$

the summation being over all n such that (k_{xn}, k_{yn}) lies in the area $dk_x dk_y$ around (k_x, k_y). From equations (11) and (23), we see that

$$m_{00} = \sigma^2 = {}^1/_2 \sum_{\text{all } n} C_n^2. \quad (24)$$

Similarly, we have

$$m_{pq} = {}^1/_2 \sum_{\text{all } n} k_{xn}^p k_{yn}^q C_n^2. \quad (25)$$

Define the variables $\xi_1 \ldots \xi_6$ as follows:

$$\left.\begin{aligned} \xi_1 &= z & \xi_4 &= \partial^2 z/\partial x^2 \\ \xi_2 &= \partial z/\partial x & \xi_5 &= \partial^2 z/\partial x \partial y \\ \xi_3 &= \partial z/\partial y & \xi_6 &= \partial^2 z/\partial y^2. \end{aligned}\right\} \quad (26)$$

The variables $\xi_1 \ldots \xi_6$ satisfy the requirements of the central limit theorem, and their joint probability density is given by equation (17). Then the matrix N_{ij} of equation (19) is found to be

$$(N_{ij}) = \begin{pmatrix} m_{00} & 0 & 0 & -m_{20} & -m_{11} & -m_{02} \\ 0 & m_{20} & m_{11} & 0 & 0 & 0 \\ 0 & m_{11} & m_{02} & 0 & 0 & 0 \\ -m_{20} & 0 & 0 & m_{40} & m_{31} & m_{22} \\ -m_{11} & 0 & 0 & m_{31} & m_{22} & m_{13} \\ -m_{02} & 0 & 0 & m_{22} & m_{13} & m_{04} \end{pmatrix} \quad (27)$$

As an example of how the elements of N_{ij} are computed, consider the element $\overline{\xi_1\xi_4}$. From equations (22) and (26) we have

$$\overline{\xi_1\xi_4} = -\overline{\sum_{\text{all } n} C_n^2 k_{xn}^2 \cos^2\,(xk_{xn} + yk_{yn} + \epsilon_n)}. \quad (28)$$

For any one value of n, the average on the right-hand side of equation (28) is taken over ϵ_n, and we have, using equation (25),

$$\overline{\xi_1\xi_4} = -{}^1/_2 \sum_{\text{all } n} C_n^2 k_{xn}^2 = -m_{20}. \quad (29)$$

When the surface is isotropic, the matrix M_{ij} of equation (18) is found, using equation (16), to be

$$M_{ij} = \begin{bmatrix} \frac{2m_4}{\Delta_1} & 0 & 0 & \frac{3m_2}{2\Delta_1} & 0 & \frac{3m_2}{2\Delta_1} \\ 0 & \frac{1}{m_2} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{m_2} & 0 & 0 & 0 \\ \frac{3m_2}{2\Delta_1} & 0 & 0 & \frac{9\Delta_2}{4m_4\Delta_1} & 0 & -\frac{3\Delta_3}{4m_4\Delta_1} \\ 0 & 0 & 0 & 0 & \frac{3}{m_4} & 0 \\ \frac{3m_2}{2\Delta_1} & 0 & 0 & -\frac{3\Delta_3}{4m_4\Delta_1} & 0 & \frac{9\Delta_2}{4m_4\Delta_1} \end{bmatrix}, \quad (30)$$

where

$$\Delta_1 = (2m_0m_4 - 3m_2^2), \quad (31)$$

$$\Delta_2 = (m_0m_4 - m_2^2), \quad (32)$$

and

$$\Delta_3 = (m_0m_4 - 3m_2^2). \quad (33)$$

The determinant Δ of N_{ij} is found to be

$$\Delta = \tfrac{4}{27}\,(m_2m_4)^2(2m_0m_4 - 3m_2^2). \quad (34)$$

Thus the joint probability distribution of the variables $\xi_1 \ldots \xi_6$ is found from equation (17) to be

$$p(\xi_1 \ldots \xi_6) = (2\pi)^{-3}\Delta^{-1/2} \exp\,(-{}^1/_2 X), \quad (35)$$

where Δ is given by equation (34) and

$$X = \frac{2m_4}{\Delta_1}\xi_1^2 + \frac{9\Delta_2}{4m_4\Delta_1}(\xi_4^2 + \xi_6^2) + \frac{3}{m_4}\xi_5^2 + \frac{3m_2}{\Delta_1}\xi_1(\xi_4 + \xi_6) - \frac{3\Delta_3}{2m_4\Delta_1}\xi_4\xi_6 + \frac{1}{m_2}(\xi_2^2 + \xi_3^2). \quad (36)$$

We shall now obtain the following statistics of the surface:

1 the probability distribution for summit heights
2 the spatial density of summits
3 the probability distribution for the mean curvature of the summits.

Distribution of Summit Heights. The requirements for some point (x, y) in an area $dA = dxdy$ to be a summit (i.e., a maximum) are that, at (x, y),

$$\left.\begin{aligned} &\xi_2 = \xi_3 = 0 \\ &\xi_4 < 0, \quad \xi_6 < 0, \quad \xi_4\xi_6 - \xi_5^2 \geq 0. \end{aligned}\right\} \tag{37}$$

The probability that the variables ξ_i at (x, y) will lie in the range $(\xi_1, \xi_1 + d\xi_1)$ is $p(\xi_1 \ldots \xi_6)d\xi_1 \ldots d\xi_6$. The increments $d\xi_2$ and $d\xi_3$ that take place in an area dA are given by

$$d\xi_2 d\xi_3 = \left|\frac{\partial(\xi_2, \xi_3)}{\partial(x, y)}\right| dA, \tag{38}$$

where the Jacobian has the value

$$\frac{\partial(\xi_2, \xi_3)}{\partial(x, y)} = \frac{\partial\xi_2}{\partial x} \cdot \frac{\partial\xi_3}{\partial y} - \frac{\partial\xi_2}{\partial y} \cdot \frac{\partial\xi_3}{\partial x} = \xi_4\xi_6 - \xi_5^2. \tag{39}$$

The point (x, y) will be a summit of height between ξ_1 and $\xi_1 + d\xi_1$ if $\xi_2 = \xi_3 = 0$, $d\xi_2$ and $d\xi_3$ satisfy equation (38) and ξ_4, ξ_5, ξ_6 take on arbitrary values subject to equation (37). Thus, if $P_{sum}(\xi_1)$ is the probability distribution for summits of height ξ_1, the probability of having a summit in the area dA with height in the range $(\xi_1, \xi_1 + d\xi_1)$ is

$$P_{sum}(\xi_1)dAd\xi_1 = d\xi_1 \times \iiint_V p(\xi_1, 0, 0, \xi_4, \xi_5, \xi_6)d\xi_2 d\xi_3 d\xi_4 d\xi_5 d\xi_6. \tag{40}$$

The domain of integration V is defined by

$$\xi_4 < 0, \quad \xi_6 < 0, \quad \xi_4\xi_6 - \xi_5^2 \geq 0. \tag{41}$$

Using equations (38) and (39) in equation (40), and substituting for $p(\xi_1 \ldots \xi_6)$ from equation (35), we obtain

$$P_{sum}(\xi_1) = \frac{\exp(-m_4\xi_1^2/\Delta_1)}{(2\pi)^3\Delta^{1/2}} \iiint_V |\xi_4\xi_6 - \xi_5^2| \exp \left\{-1/2\left[\frac{9\Delta_2}{4m_4\Delta_1} \times (\xi_4^2 + \xi_6^2) + \frac{3}{m_4}\xi_5^2 + \frac{3m_2}{\Delta_1}\xi_1(\xi_4 + \xi_6) - \frac{3\Delta_3}{2m_4\Delta_1}\xi_4\xi_6\right]\right\} d\xi_4 d\xi d\xi_6. \tag{42}$$

Define

$$\left.\begin{aligned} &(t_1, t_2, t_3) = \left(\frac{3}{m_4}\right)^{1/2} [1/2(\xi_4 + \xi_6), \xi_5, 1/2(\xi_4 - \xi_6)] \\ &\text{and} \\ &\xi_1^* = \xi_1/m_0^{1/2} = \xi_1/\sigma. \end{aligned}\right\} \tag{43}$$

Then, using the transformation $P_{sum}(\xi_1^*) = P_{sum}(\xi_1)|\partial\xi_1/\partial\xi_1^*|$, equation (43) may be written

$$P_{sum}(\xi^*) = \left(\frac{m_4}{m_2}\right) \frac{[C_1(\alpha)]^{1/2}}{3(2\pi)^3} \exp[-C_1\xi^{*2}] \times \iiint_{V'} |t_1^2 - t_2^2 - t_3^2| \exp\{-1/2 [C_1t_1^2 + t_2^2 + t_3^2 + C_2t_1\xi^*]\} dt_1dt_2dt_3, \tag{44}$$

where

$$\left.\begin{aligned} &\alpha = m_0m_4/m_2^2 \\ &C_1 = \alpha/(2\alpha - 3) \\ &\text{and} \\ &C_2 = C_1(12/\alpha)^{1/2}. \end{aligned}\right\} \tag{45}$$

The domain of integration V' is defined by

$$\left.\begin{aligned} &t_1 < 0 \\ &t_2^2 + t_3^2 \leq t_1^2. \end{aligned}\right\} \tag{46}$$

The probability density for summit heights, p_{sum} is obtained by dividing P_{sum} by D_{sum}, the density of summits:

$$p_{sum}(\xi^*) = P(\xi_{sum}^*)/D_{sum}, \tag{47}$$

where

$$D_{sum} = \int_{-\infty}^{\infty} P_{sum}(\xi^*)d\xi^*. \tag{48}$$

The integrals in equations (44) and (48) may be evaluated analytically to yield

$$D_{sum} = \frac{1}{6\pi\sqrt{3}} \left\{\frac{m_4}{m_2}\right\}. \tag{49}$$

This result agrees with the expression given by Longuet-Higgins [3], which was derived by a slightly different method.

Substituting the expression for D_{sum} into equation (47), we obtain

$$p_{sum}(\xi^*) = \frac{\sqrt{3}}{2\pi}\left\{e^{-C_1\xi^{*2}}\left[\frac{3(2\alpha - 3)}{\alpha^2}\right]^{1/2} + \frac{3\sqrt{2\pi}}{2\alpha} e^{-1/2\xi^{*2}} (1 + \text{erf}\,\beta)(\xi^{*2} - 1) + \sqrt{2\pi}\left[\frac{\alpha}{3(\alpha - 1)}\right]^{1/2} \exp\{-[(\alpha\xi^{*2})/2(\alpha - 1)]\} \times (1 + \text{erf}\,\gamma)\right\}, \tag{50}$$

where

$$\left.\begin{aligned} &\beta = \left[\frac{3}{2(2\alpha - 3)}\right]^{1/2}\xi^* \\ &\text{and} \\ &\gamma = \left[\frac{\alpha}{2(\alpha - 1)(2\alpha - 3)}\right]^{1/2}\xi^* \end{aligned}\right\}. \tag{51}$$

The probability density $p_{sum}(\xi^*)$ is shown in Fig. 4 for a range of values of α. Longuet-Higgins [2] has shown that $\alpha \geq 1.5$ for a random, isotropic surface. Thus no values of α lower than 1.5 appear in Fig. 4. It may be seen that as α decreases to 1.5, the probability of a high peak increases. The parameter α is related to the breadth of the surface PSD. A broad spectrum is one that has waves with a large range of wavelengths; a narrow spectrum has waves of approximately equal wavelength. As $\alpha \rightarrow 1.5$, the spectrum gets narrower; and as $\alpha \rightarrow \infty$, it gets broader.

The two limiting forms of p_{sum} for $\alpha \rightarrow 1.5$ and $\alpha \rightarrow \infty$ are:

1 *Lim* $\alpha \rightarrow 1.5$

$$p_{sum}(\xi^*) = \begin{cases} \dfrac{2\sqrt{3}}{\sqrt{2\pi}} e^{-1/2\xi^{*2}} [\xi^{*2} - 1 + e^{-\xi^{*2}}], & \xi^* \geq 0 \\ 0, & \xi^* < 0. \end{cases} \tag{52}$$

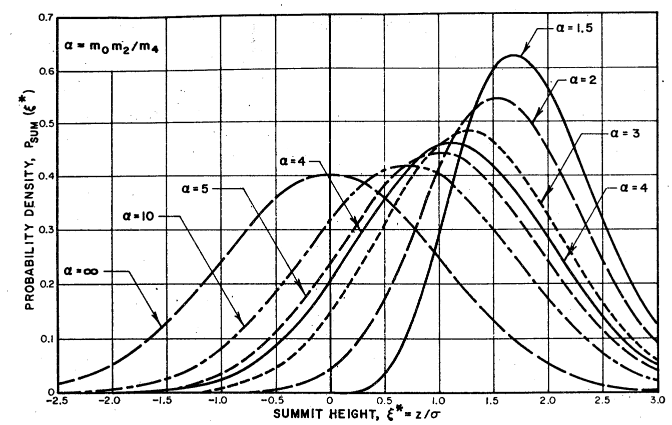

Fig. 4 Probability density for summit heights

Table 1 Cumulative probability distribution for summit heights

ξ^*	$q_{sum} = \int_{-\infty}^{\xi^*} P_{sum}(\xi^*)d\xi^*$						
	$\alpha = 1.5$	2	3	4	5	10	∞
0.0	0.0	.0129	.0601	.1026	.1363	.2327	.5
.25	.0001	.0306	.1103	.1686	.2118	.3263	.5987
.50	.0037	.0706	.1739	.2446	.2943	.4187	.6915
.75	.0237	.1296	.2696	.3496	.4031	.5296	.7733
1.00	.0785	.2281	.3701	.4521	.5050	.6251	.8413
1.25	.1787	.3381	.4955	.5724	.6205	.7251	.8943
1.50	.3176	.4794	.6052	.6724	.7134	.8000	.9332
1.75	.4745	.6030	.7199	.7725	.8040	.8689	.9599
2.00	.6254	.7293	.8042	.8435	.8668	.9138	.9772
2.25	.7525	.8187	.8785	.9044	.9196	.9498	.9878
2.50	.8482	.8936	.9247	.9414	.9512	.9704	.9938
2.75	.9134	.9375	.9594	.9687	.9742	.9848	.9970
3.00	.9539	.9625	.9778	.9830	.9861	.9920	.9987

2 *Lim* $\alpha \rightarrow \infty$

$$p_{sum}(\xi^*) = \frac{1}{\sqrt{2\pi}} e^{-1/2\xi^{*2}}. \tag{53}$$

Thus, when $\alpha \rightarrow \infty$, the summit heights have a Gaussian distribution. When $\alpha \rightarrow 1.5$, the distribution of summit heights *for* $\xi^* > 2$ may be written

$$p_{sum}(\xi^* > 2) \approx \left(\frac{6}{\pi}\right)^{1/2} (\xi^{*2} - 1)e^{-1/2\xi^{*2}}, \quad \alpha = 1.5. \tag{54}$$

The most remarkable thing about the expression for $p_{sum}(\xi^*)$ is that it depends only on the parameter α, which may be obtained from a surface profile, as explained in Section 4.

An interesting observation that may be made about the expected density of summits D_{sum} (#/unit area), equation (49), is that when the surface PSD is flat up to fairly high wavenumbers (i.e., small wavelengths), D_{sum} will be very large. This is because one effect of the small-wavelength components is to cause large clusters of "mini-summits" of small amplitude and wavelength to appear around a "maxi-summit" of large amplitude and wavelength. If, however, one is interested only in the maxi-summits, their density may be obtained by filtering out the high wave-number content of the surface PSD. This causes m_4 to decrease faster than m_2, and consequently causes a decrease in D_{sum}.

A further quantity of interest is the cumulative density of summits $q_{sum}(\xi^*)$, which indicates the fraction of all summits that are expected to lie below ξ^*:

$$q_{sum}(\xi^*) = \int_{-\infty}^{\xi^*} p_{sum}(\xi^*)d\xi^*. \tag{55}$$

This function is tabulated in Table 1. It may be seen that as $\alpha \rightarrow 1.5$, the fraction of summits that lie below the $+3\sigma$ level (i.e., below $\xi^* = 3$) decreases.

The Mean Summit Curvature. The mean curvature κ_m at any point on a surface is defined as the mean of the principal curvatures κ_1 and κ_2 at that point. In addition, the sum of the curvatures of a surface at a point along any two orthogonal directions is equal to the sum of the principal curvatures [9]. Furthermore, the curvatures of a surface at a summit in the x and y directions are $-\partial^2z/\partial x^2$ and $-\partial^2z/\partial y^2$. Thus the mean curvature at a summit is

$$\kappa_m = 1/2(\kappa_1 + \kappa_2) = -\frac{1}{2}\left(\frac{\partial^2z}{\partial x^2} + \frac{\partial^2z}{\partial y^2}\right) = -\frac{1}{2}(\xi_4 + \xi_6). \tag{56}$$

Using equation (43), we find

$$\kappa_m = -\left(\frac{m_4}{3}\right)^{1/2} t_1. \tag{57}$$

We call t_1 the equivalent mean curvature. The joint probability distribution for summits with height ξ_1^* and equivalent mean curvature t_1 is

$$P_{sum}(\xi_1^*, t_1) = \frac{\left(\frac{m_4}{m_2}\right)}{3(2\pi)^3} C_1^{1/2} \exp[-C_1\xi^{*2}] \times \exp\{-1/2[C_1(\alpha)t_1^2 + C_2(\alpha)t_1\xi^*]\} \times \iint_S |t_1^2 - t_2^2 - t_3^2| \exp\{-1/2[t_2^2 + t_3^2]\} dt_2dt_3. \tag{58}$$

The domain of integration S is defined by

$$t_1^2 \geq t_2^2 + t_3^2. \tag{59}$$

In addition, at a summit we always have $t_1 < 0$.

$P_{sum}(\xi_1^*, t_1)$ may be normalized by dividing by D_{sum} to yield a probability density:

$$p_{sum}(\xi_1^*, t_1) \equiv P_{sum}(\xi_1^*, t_1)/D_{sum}. \tag{60}$$

The integral in equation (58) may be evaluated analytically to give

$$p_{sum}(\xi_1^*, t_1) = \frac{\sqrt{3C_1}}{2\pi} \exp(-C_1\xi^{*2}) \times (t_1^2 - 2 + 2e^{-1/2t_1^2}) \exp\{-1/2[C_1(\alpha)t_1^2 + C_2(\alpha)t_1\xi^*]\}. \tag{61}$$

The expected value of the mean curvature for summits of height ξ_1^*, $\bar{\kappa}_m(\xi_1^*)$ is found from equation (61):

$$\bar{\kappa}_m(\xi_1^*) = \frac{-\left(\frac{m_4}{3}\right)^{1/2} \int_{-\infty}^{0} t_1 p_{sum}(\xi_1^*, t_1)dt_1}{\int_{-\infty}^{0} p_{sum}(\xi_1^*, t_1)dt_1} \tag{62}$$

The expression for $\bar{\kappa}_m(\xi^*)$ is found analytically to be

$$\bar{\kappa}_m(\xi^*) = \left(\frac{m_4}{3}\right)^{1/2} \cdot \frac{I_3(\xi^*) - 2I_1(\xi^*) + 2I_5(\xi^*)}{I_2(\xi^*) - 2I_0(\xi^*) + 2I_4(\xi^*)}, \tag{63}$$

where $I_0 \ldots I_5$ are functions of ξ^* and α, given in Appendix 1.

The dimensionless expected mean curvature $\bar{\kappa}_m/\sqrt{m_4}$ is shown in Fig. 5 for a range of values of α. It may be seen that high peaks always have a larger expected mean curvature (i.e., a smaller summit radius) than lower peaks. For $\alpha = 1.5$, $\bar{\kappa}_m$

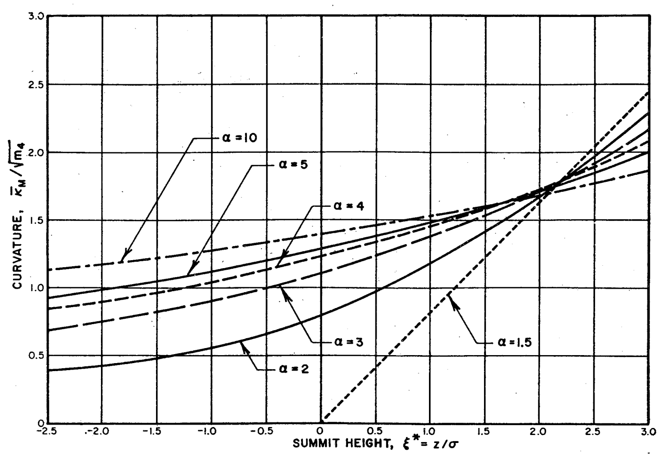

Fig. 5 Expected mean dimensionless curvature of summits

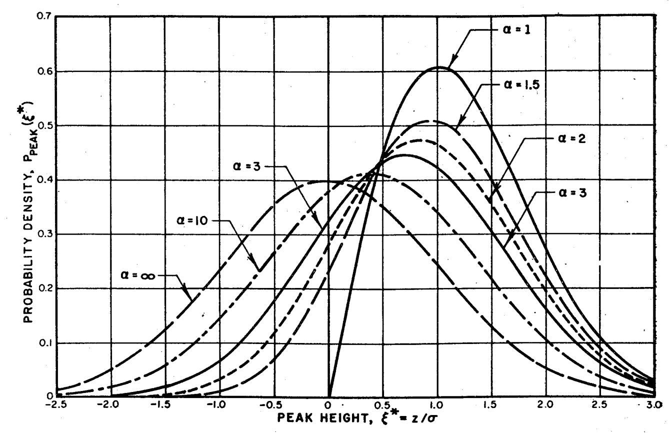

Fig. 6 Probability density for heights of peaks on a profile

varies linearly with ξ^*. For very large values of α, however, the expected mean curvature is very nearly constant for summits of all heights. The two limiting cases are:

1 *Lim* $\alpha \rightarrow 1.5$

$$\bar{\kappa}_m/\sqrt{m_4} = \sqrt{2/3}\,\xi^*, \qquad \xi^* \geq 0. \tag{64}$$

2 *Lim* $\alpha \rightarrow \infty$

$$\bar{\kappa}_m/\sqrt{m_4} = 8/3\sqrt{\pi}. \tag{65}$$

Further fairly elementary results may be derived concerning the probability distributions of the height of the surface and the surface gradient.

The Surface Height. The probability density for the surface height ξ_1 is obtained in a straightforward manner from equation (17) by noting that

$$M_{11} = \frac{1}{N_{11}} = \frac{1}{\bar{\xi}_1^2} = \frac{1}{m_{00}} = \frac{1}{\sigma^2},$$

and $\Delta = \sigma^2$. Thus,

$$p(\xi_1) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-{}^1/_2(\xi_1/\sigma)^2\right]. \tag{66}$$

The Surface Gradient. The surface gradient is defined by

$$\zeta = (\xi_2^2 + \xi_3^2)^{1/2}. \tag{67}$$

Longuet-Higgins [10] shows that the probability density for ζ is

$$p(\zeta) = \frac{\zeta}{m_2} \exp\left(-\zeta^2/2m_2\right). \tag{68}$$

The expected value of the gradient is found from equation (68)

$$\bar{\zeta} = \int_0^\infty \zeta p(\zeta) d\zeta = \left(\frac{\pi m_2}{2}\right)^{1/2}. \tag{69}$$

4 The Sampling of Random Surfaces

In Section 3, it was shown that a large number of useful statistics of the surfaces may be found for random, isotropic, Gaussian surfaces if the parameters m_0, m_2, and m_4 are known. It was also shown that these parameters are moments of the PSD of a profile of the surface in an arbitrary direction.

Once a profile of the surface is obtained, the autocorrelation of the profile may be calculated, using equation (7). The profile PSD is then calculated, using equation (8). The moments m_0, m_2, and m_4 are obtained by using equation (13).

An ingenious alternative has been described by Longuet-Higgins [2]. He shows that the densities of zeroes and of extrema (maxima or minima) along a profile are given by

$$D_{\text{zero},\,\theta} = \frac{1}{\pi}\left(\frac{m_2}{m_0}\right)^{1/2}, \tag{70}$$

and

$$D_{\text{extrema},\,\theta} = \frac{1}{\pi}\left(\frac{m_4}{m_2}\right)^{1/2}. \tag{71}$$

The subscript θ indicates a profile statistic, not anistropy.

Once a profile is obtained, $\sigma = \sqrt{m_0}$ is easily calculated. Then m_2 and m_4 may be obtained from equations (70) and (71) simply by counting the number of zeroes and extrema per unit length of the profile:

$$m_2 = \pi^2\sigma^2(D_{\text{zero},\,\theta})^2, \tag{72}$$

and

$$m_4 = \pi^4\sigma^2(D_{\text{zero},\,\theta})^2(D_{\text{extrema},\,\theta})^2. \tag{73}$$

It is worth noting that by this technique, the high wavenumber content of Φ_θ is filtered out if one only counts major peaks, valleys, and zero-crossings. Conversely, a low-pass filtered signal will only contain major peaks, valleys, and zero-crossings.

The parameter α of equation (45) is

$$\alpha = \frac{m_0 m_4}{m_2^2} = \left(\frac{D_{\text{extrema},\,\theta}}{D_{\text{zero},\,\theta}}\right)^2. \tag{74}$$

In passing, we may note that the density of peaks (maxima) along the profile is, due to symmetry, one-half the number of extrema:

$$D_{\text{peak}} = \frac{1}{2\pi}\left(\frac{m_4}{m_2}\right)^{1/2}. \tag{75}$$

Comparing this with the density of summits on the surface, D_{sum}, equation (49), we have

$$D_{\text{sum}} \approx 1.2(D_{\text{peak}})^2. \tag{76}$$

The question arises as to whether the parameters m_0, m_2, m_4, and α can be obtained in a direct fashion by instrumental analysis of the output of a profilometer. One technique for doing this, being developed at Bolt Beranek and Newman Inc., is as follows. The signal from the profilometer is passed through a preamplifier, low-pass filter with adjustable cutoff frequency, and an amplifier. The rms value is read directly from a quasi-rms meter. A circuit for determining the zero-level of the signal is used along with a comparator and a counter to determine the zero-crossing rate. To obtain the rate of extrema, the zero-crossing rate of the differentiated signal is measured. The cutoff frequency on the filter is adjusted according to the nature of the particular contact problem being investigated.

For further comparisons between the statistics of the surface and the statistics of the profile, we present results for (*a*) the height distribution of peaks of the profile, (*b*) the expected value of the peak curvature as a function of peak height, and (*c*) the distribution of slopes on the profile.

Heights of Profile Peaks Cartwright and Longuet-Higgins [11], following Rice [12], have shown that the probability density for the heights of profile peaks is

$$p_{\text{peak}}(\xi^*) = \frac{\delta}{\sqrt{2\pi}}\left\{\exp\left[-(\xi^{*2}/2\delta^2)\right] + \sqrt{\pi}\,\chi \exp\left(-{}^1/_2\,\xi^{*2}\right)(1 + \text{erf}\,\chi)\right\}, \tag{77}$$

where

$$\left.\begin{aligned} \alpha &= m_0 m_4/m_2^2 \\ \delta &= [(\alpha - 1)/\alpha]^{1/2} \\ \text{and} \quad \chi &= \left(\frac{1-\delta^2}{2\delta^2}\right)^{1/2}\xi^* \end{aligned}\right\}. \tag{78}$$

The function $p_{\text{peak}}(\xi^*)$ is shown in Fig. 6 for a range of values of α. It may be shown that for one-dimensional random processes, $1 \leq \alpha \leq \infty$. Thus, δ varies from $\delta = 0$ when $\alpha = 1$ to $\delta = 1$ when $\alpha = \infty$. The significance of the parameter α is the same as for a random surface. Small values of α indicate a narrow spectrum, and large values of α indicate a broad spectrum. When the one-dimensional random process is a profile of an isotropic, random surface, however, α can only take values greater than 1.5.

Figs. 7–9 show a comparison of $p_{\text{peak}}(\xi^*)$ and $p_{\text{sum}}(\xi^*)$. It may be seen that the profile distorts the surface in such a way as to show far fewer high peaks and far more low peaks than actually exist on the surface. The distortion is the greatest when $\alpha = 1.5$; it becomes zero when $\alpha \rightarrow \infty$. The reason for the distortion is that more often than not, the profile-measuring instrument will travel over the shoulder of an asperity on the surface, rather than over the summit. A peak will still appear on the profile, but of a smaller height than the summit being sampled.

In the limiting cases of $\alpha \rightarrow 1$ and $\alpha \rightarrow \infty$, the following expressions are obtained for p_{peak} from equation (77):

1 *Lim* $\alpha \rightarrow 1$

Table 2 Cumulative probability distribution for peak heights

ξ^*	$q_{\text{peak}} = \int_{-\infty}^{\xi^*} p_{\text{peak}}(\xi^*)d\xi^*$							
	α = 1.0	1.5	2	3	4	5	10	∞
0.0	0.0	.0956	.1560	.2168	.2558	.2823	.3482	.5
.25	.0308	.1738	.2340	.3143	.3568	.3853	.4541	.5987
.50	.1175	.2662	.3434	.4119	.4545	.4827	.5497	.6915
.75	.2452	.3923	.4506	.5296	.5690	.5948	.6552	.7733
1.00	.3935	.5105	.5760	.6304	.6647	.6870	.7388	.8413
1.25	.5422	.6410	.6789	.7348	.7617	.7792	.8196	.8943
1.50	.6754	.7314	.7804	.8115	.8320	.8452	.8757	.9332
1.75	.7837	.8335	.8510	.8800	.8938	.9027	.9233	.9599
2.00	.8648	.8932	.9104	.9235	.9326	.9386	.9522	.9772
2.25	.9204	.9398	.9458	.9571	.9624	.9659	.9738	.9878
2.50	.9561	.9656	.9714	.9756	.9787	.9807	.9854	.9938
2.75	.9772	.9830	.9846	.9880	.9895	.9905	.9929	.9970
3.00	.9889	.9910	.9929	.9939	.9947	.9952	.9964	.9987

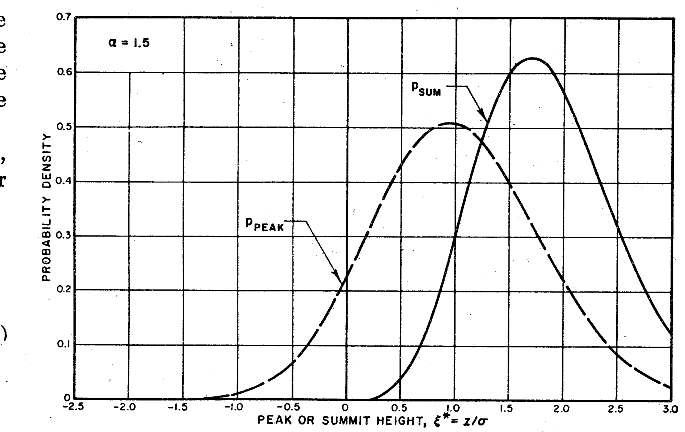

Fig. 7 Comparison of probability densities for peak and summit heights

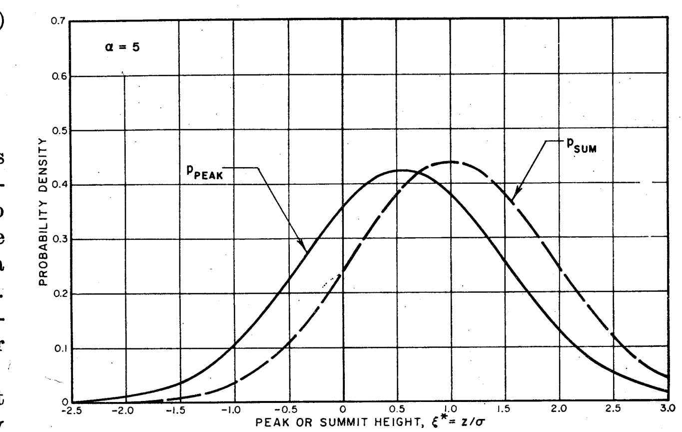

Fig. 8 Comparison of probability densities for peak and summit heights

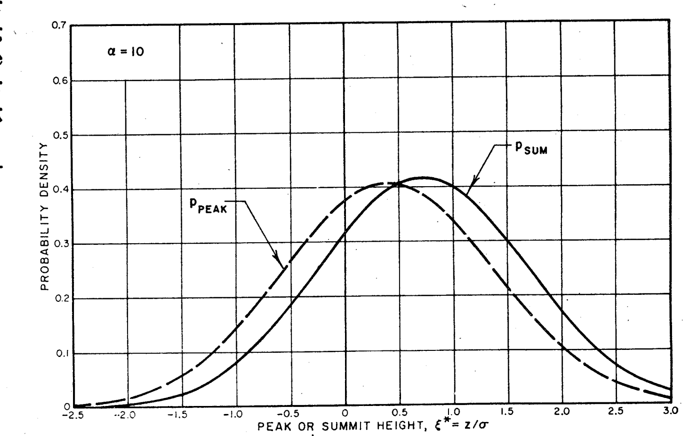

Fig. 9 Comparison of probability densities for peak and summit heights

$$p_{\text{peak}}(\xi^*) = \begin{cases} \xi^* \exp\left(-{}^1/_2\xi^{*2}\right), & \xi^* \geq 0 \\ 0, & \xi^* < 0. \end{cases} \tag{79}$$

2 *Lim* $\alpha \rightarrow \infty$

$$p_{\text{peak}}(\xi^*) = \frac{1}{\sqrt{2\pi}} \exp\left(-{}^1/_2\xi^{*2}\right). \tag{80}$$

The cumulative probability density for peak heights,

$$q_{\text{peak}}(\xi^*) = \int_{-\infty}^{\xi^*} p_{\text{peak}}(\xi^*)d\xi^*, \tag{81}$$

is tabulated in Table 2. It is clear from a comparison of the data

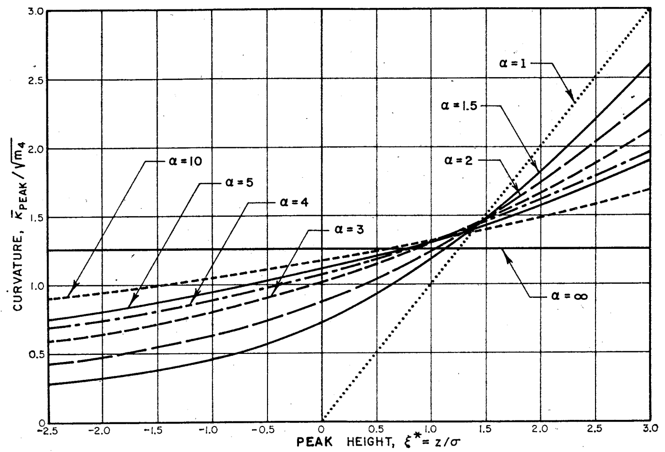

Fig. 10 Expected value of dimensionless tip curvature of peaks on a profile

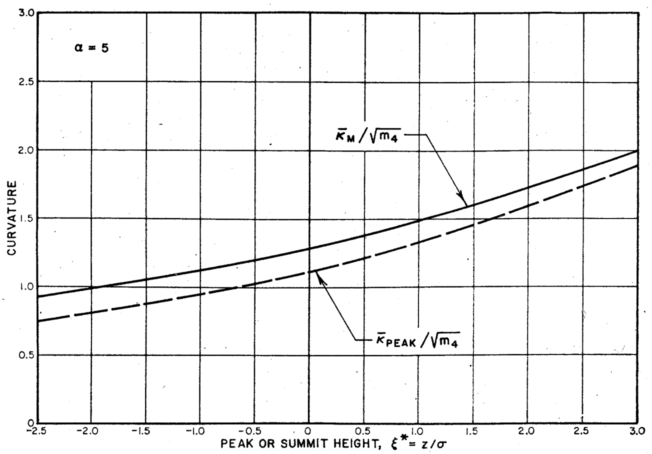

Fig. 12 Comparison of expected summit and peak curvatures

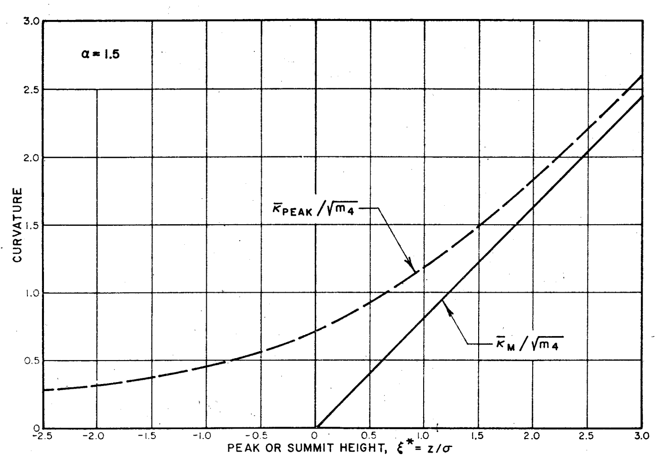

Fig. 11 Comparison of expected summit and peak curvatures

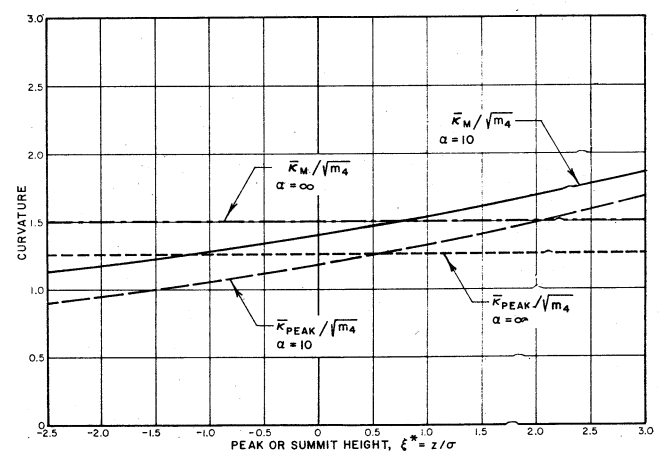

Fig. 13 Comparison of expected summit and peak curvatures

in Tables 1 and 2 that there are many more summits above the $+3\sigma$ level than would be indicated by the profile, except when $\alpha \rightarrow \infty$.

Peak Curvature. In a manner similar to that leading to the expected mean summit curvature, $\bar{\kappa}_m(\xi^*)$, equation (63), the expected value of the profile peak curvature is found to be

$$\bar{\kappa}_{\text{peak}}(\xi^*) = m_4^{1/2}\delta\sqrt{2}\,\frac{[\chi + \sqrt{\pi}\, e^{\chi^2}(1+\text{erf}\chi)(\chi^2+0.5)]}{[1+\chi\, e^{\chi^2}\sqrt{\pi}\,(1+\text{erf}\chi)]}, \quad (82)$$

where δ and χ are as defined in equation (78).

The dimensionless peak curvature $\bar{\kappa}_{\text{peak}}/\sqrt{m_4}$ is shown in Fig. 10. Figs. 11–13 show a comparison of $\bar{\kappa}_{\text{peak}}/\sqrt{m_4}$ and $\bar{\kappa}_m/\sqrt{m_4}$. The distortion of the surface by the profile is again evident, but is now quite small for $\alpha > 2$. For $\alpha \lesssim 2.5$, the profile shows a larger peak curvature than the true summit curvature. For $\alpha > 2.5$, the profile peak curvature is less than the summit curvature.

The Profile Slope. Consider a profile taken along the x axis. The height of the profile is $\xi_1 = z$ and the slope is $\xi_2 = \partial z/\partial x$. The joint probability density for ξ_1 and $\xi_2 = \partial z/\partial x$ is found from equation (17) to be

$$p(\xi_1, \xi_2) = p(\xi_1)p(\xi_2), \quad (83)$$

since $\overline{\xi_1\xi_2} = 0$. $p(\xi_2)$ is found, by the techniques detailed in Section 3 to be

$$p(\xi_2) = \frac{1}{\sqrt{2\pi m_2}} \exp\,[-\xi_2^2/2m_2]. \quad (84)$$

Equation (83) indicates that the probability density for surface slopes in a given direction is statistically independent of the surface elevation at which the slope is measured. From equation (84), the expected value of the absolute slope $\overline{|\xi_2|}$ at any elevation is

$$\overline{|\xi_2|} = \left(\frac{2}{\pi m_2}\right)^{1/2}\int_0^\infty \xi_2 \exp\,(-{}^1\!/_2\xi_2^2/m_2)d\xi_2 = \left(\frac{2m_2}{\pi}\right)^{1/2}. \quad (85)$$

Similar comments apply to ξ_3, the surface slope in the direction of the y axis.

A comparison of equations (69) and (85) indicates that the mean gradient on the surface is always larger than the mean slope on the profile:

$$\bar{\zeta} = \frac{\pi}{2}\overline{|\xi_2|} = \frac{\pi}{2}\overline{|\xi_3|}. \quad (86)$$

5 Discussion

Whitehouse and Archard [13] have recently provided a detailed discussion of three-point analyses of surface profiles. We shall briefly examine the connection between their work and ours. Their theory assumes an autocorrelation function of the form

$$R(r) = m_0 \exp\,(-\beta|r|), \quad (87)$$

where β is a factor governing the swiftness of decay of the correlation. Using equation (8), the profile PSD is found to be

$$\Phi(k') = \frac{m_0}{2\pi}\cdot\frac{2\beta}{\beta^2 + k'^2} \quad (88)$$

It may be seen that when β is large, the autocorrelation decays swiftly, and the PSD is almost flat out to large values of k'. We may now attempt to obtain the parameters m_2 and m_4, using equation (13). Upon introducing equation (88) into equation (13), however, we find a result that is well-known in the theory of Markov processes: for a random process with an exponential autocorrelation function, the mean-square slope (m_2) and the mean-square second derivative (m_4) are undefined. This can be traced directly to the fact that for an exponential autocorrelation function, equation (87), the second and fourth derivatives are undefined at $x = 0$. The relation inverse to equation (8) is

$$R(r) = \int_{-\infty}^{\infty} \Phi(k') \exp\,(ik'r)dk'. \quad (89)$$

Differentiating equation (89) and combining it with equation (13), we obtain

$$\left(\frac{d^2R}{dr^2}\right)_{r=0} = -\int_{-\infty}^{\infty} (k')^2\Phi(k')dk' = -m_2 \quad (90)$$

and

$$\left(\frac{d^4R}{dr^4}\right)_{r=0} = -\int_{-\infty}^{\infty} (k')^4\Phi(k')dk' = m_4 \quad (91)$$

Thus, in order for the parameters m_2 and m_4 (and therefore α) to exist, the autocorrelation function must be smooth at the origin, in the sense that its second and fourth derivatives exist. It is entirely likely that $R(r)$ is exponential for large r; however, extrapolation of this behavior to small values of r is manifestly unsafe. There is thus an inherent theoretical contradiction in Whitehouse and Archard's work: their mathematical model does not allow slopes and curvatures to exist, though they proceed to obtain these data from profiles. The reason why this does not amount to a contradiction in practice is that their sampling interval is finite; the effect of a finite sampling interval being to filter out small-wavelength components, and to change the behavior of the autocorrelation function at the origin.

In order to examine the consequences of this filtering out of small wavelengths (i.e., large wave-numbers), consider a profile PSD of the form

$$\Phi(k') = \begin{cases} \dfrac{C}{\beta^2 + k'^2}, & |k'| \le k_0 \\ 0, & |k'| > k_0 \end{cases} \quad (92)$$

Using equation (13), we find

$$m_0 = \frac{2C}{\beta}\tan^{-1}(k_0/\beta),$$

$$m_2 = 2C[k_0 - \beta\tan^{-1}(k_0/\beta)] \quad (93)$$

and

$$m_4 = 2C\left[\frac{k_0^3}{3} - \beta^2 k_0 + \beta^3\tan^{-1}(k_0/\beta)\right].$$

The parameter α can now be obtained from equation (45), and is found to be

$$\alpha = \tan^{-1} A\,[\tfrac{1}{3}A^3 - A + \tan^{-1} A]/(A - \tan^{-1}A)^2, \quad (94)$$

where

$$A = (k_0/\beta). \quad (95)$$

It may be seen that $\alpha \rightarrow \infty$ as $A \rightarrow \infty$. In this limit, the peak-height distribution is found from Fig. 6 to be Gaussian, a result that agrees with that of Whitehouse and Archard [13]. For other values of A, α may be obtained from equation (95); profile and surface statistics may then be obtained with the techniques described in this paper.

6 Conclusions

To reiterate the main theoretical theme of this paper, the extremal statistics of a random surface must be distinguished from the statistics of a profile of the surface. All the information necessary for the analysis of random, isotropic, Gaussian surfaces is contained in the power spectral density of a profile in an arbitrary direction. The analytical techniques for obtaining the statistics of the surface are given in Section 3. A simple technique for obtaining the parameters necessary for this analysis is described in Section 4.

In general, it is found that the profile, if interpreted simplistically, indicates a lower probability for high summits, a smaller summit curvature, and a smaller mean gradient than actually exist on the surface. The implications of this distortion for problems involving contact of rough surfaces is obvious.

It may be noted that the theory outlined in this paper is, in principle, easy to extend to nonisotropic Gaussian surfaces. The development of the theory remains valid up to equation (27); beyond this point, it is necessary to do without the use of equations (16), which imply isotropy. Longuet-Higgins gives the density of summits for nonisotropic Gaussian surfaces [2], and discusses in detail surface slopes and gradients [10]. However, results are not available for probability densities for summit heights and mean curvatures.

An interesting fact about nonisotropic surfaces is that one needs nine constants to proceed with an analysis analogous to ours: m_{00}, m_{20}, m_{02}, m_{11}, m_{13}, m_{31}, m_{22}, m_{40}, and m_{04}. However, the properties of the surface we are concerned with are independent of the orientation of the x-y axes on the surface. Thus only certain invariant combinations of the moments m_{ij} appear in the probability distributions of the surface statistics. Longuet-Higgins [10] has shown that for $(i + j) \le 4$, there are only seven such invariants. These are m_{00}, $(m_{02} + m_{20})$, $(m_{20}m_{02} - m_{11})^2$, $(m_{40} + 2m_{22} + m_{04})$, $(m_{40}m_{04} - 4m_{13}m_{31} + 3m^2_{22})$, $(m_{40} + m_{22})(m_{22} + m_{04}) - (m_{31} + m_{13})^2$ and $m_{40}(m_{22}m_{04} - m^2_{13}) - m_{31}(m_{31}m_{04} - m_{13}m_{22}) + m_{22}(m_{31}m_{13} - m^2_{22})$.

For a profile along any direction θ, three equations may be written for the profile moments $m_{0\theta}$, $m_{2\theta}$, and $m_{4\theta}$ in terms of the m_{ij}, as in equation (14). For three profiles, nine such equations may be written, but three of these (involving m_{00}) are linearly dependent, leaving seven independent equations from which the seven invariants may be obtained.

A final observation that may be made is that all the higher-order surface statistics of interest depend only on the parameters m_0, m_2, and m_4, obtained from a single profile for Gaussian, isotropic surfaces, and from three nonparallel profiles for Gaussian, nonisotropic surfaces. Therefore, it seems worthwhile to investigate the possibility of defining the surface finish of solids by these three parameters. The suggestion is particularly attractive because of the ease with which the three parameters may be obtained from a profile, as described in Section 4.

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APPENDIX 1

The expressions $I_0 \ldots I_5$ appearing in equation (63) are as follows:

$$I_0 = \left(\frac{\pi}{2C_1}\right)^{1/2} \exp\left(-{}^1/_2\xi^{*2}\right)(1 + \operatorname{erf}\beta), \qquad \text{(A1)}$$

$$I_1 = 1/C_1[\exp(-C_1\xi^{*2}) + \beta\exp(-{}^1/_2\xi^{*2})\sqrt{\pi}(1 + \operatorname{erf}\beta)], \qquad \text{(A2)}$$

$$I_2 = \sqrt{2}/C_1^{3/2}[\beta\exp(-C_1\xi^{*2}) + \sqrt{\pi}\exp(-{}^1/_2\xi^{*2}) \times (1 + \operatorname{erf}\beta)(\beta^2 + {}^1/_2)], \qquad \text{(A3)}$$

$$I_3 = 2/C_1^2[(1 + \beta^2)\exp(-C_1\xi^{*2}) + \sqrt{\pi}\exp(-{}^1/_2\xi^{*2}) \times (1 + \operatorname{erf}\beta)(\beta^3 + 3\beta/2)], \qquad \text{(A4)}$$

$$I_4 = \frac{1}{(C_1 + 1)^{1/2}} \cdot \left(\frac{\pi}{2}\right)^{1/2} \times \exp\{-[\alpha\xi^{*2}]/[2(\alpha - 1)]\}(1 + \operatorname{erf}\gamma) \qquad \text{(A5)}$$

$$I_5 = \frac{1}{C_1 + 1}[\exp(-C_1\xi^{*2}) + \gamma \times \exp\{-[\alpha\xi^{*2}]/[2(\alpha - 1)]\}\sqrt{\pi}(1 + \operatorname{erf}\gamma)], \qquad \text{(A6)}$$

C_1 being defined in equation (45), and β and γ being defined in equation (51).

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