4. Calculation of the Power Spectral Density Function and the rms Roughness

All topographic images of surfaces in this study were in the form of digitized data of surface heights, either as a 1-D profile in the form of $h(x)$ where x is the coordinate on the surface ($0 < x < L$), L is the profile length, and h is the surface height measured relative to the mean surface level; or as a 2-D array in the form of $h(x, y)$ where x and y are the coordinates on the surface. The area was in the form of a square that was restricted to the interval $0 < x, y < L$, where L is the maximum dimension and $h(x, y)$ is measured relative to the mean surface plane. The $h(x)$ and $h(x, y)$ height data were obtained from the raw height data after we corrected for offset, tilt, and curvature. The offset correction was obtained when we shifted the height of the origin so that the resulting average of all height data in a set was zero. The tilt correction eliminated possible sample inclination with respect to the mean surface plane. Curvature in the measurements could appear when the three displacement degrees of freedom of the scanning probe in an instrument such as an AFM were not completely independent. For example, curvature was observed in AFM measurements of relatively large areas (of the order of several tens of micrometers) because of the action of the piezoelectric scanner that moved the probe. We made the corrections by fitting the measured data to a polynomial by a least-squares routine and then subtracting the resulting polynomial from the measurement data. The constant term of the polynomial corresponded to the offset correction, the linear term corresponded to the tilt, and the quadratic and cubic terms corrected for the curvature.

The PSD function is customarily defined in its limiting integral form for continuous data sets as[8,9,50]

$$\mathrm{PSD}(f_x, f_y) = \lim_{L\to\infty} \frac{1}{L^2} \left| \int_{-L/2}^{L/2} \int_{-L/2}^{L/2} h(x, y) \times \exp[-2\pi i(f_x x + f_y y)]\mathrm{d}x\mathrm{d}y \right|^2, \quad (1)$$

where the surface topography data are $h(x, y)$ and the PSD variables f_x and f_y are the spatial frequencies of the surface roughness and are related to the lateral dimensions of the surface features. According to Eq. (1), the PSD gives information about the relative contributions of all the possible surface spatial frequencies for an ideal measurement of an infinite surface in the limiting case from 0 frequency (an infinite surface area) to an infinite frequency (infinitely small structures).

As was noted above, the measurements in this paper are all digitized data sets, either arrays representing topography (heights) over a surface area or profiles giving surface heights along a line on the surface. In all cases the heights were measured relative to a mean surface level that was determined in the measurement area. The PSD for digitized data in one dimension (one of the Cartesian coordinates or the radial vector in polar coordinates) can be written as[8]

$$\mathrm{PSD}(f_x)_N(m) = \left| \left(\frac{\tau_0}{N}\right) \sum_{n=0}^{N-1} h(x)_n \times \exp(-i2\pi mn/N) \right|^2 K(m), \quad (2)$$

where $-N/2 \le m \le (N/2) - 1$. Equation (2) gives an expression for the mth term in the PSD calculated from a profile of N points. There are now discrete values of $f_x = m/L$, where L is the measurement length and x in the function $h(x)_n$ takes on discrete values: $x = (L/N)\, n$. Also, τ_0 is the spacing between data points in the profile, $h(x)_n$ are the height values of the profile data points, and $K(m)$ is a bookkeeping factor that equals 1 except that $K(\pm N/2) = ½$ at the ends of the power spectrum.[51] Sometimes a data window is inserted in the summation to condition the random profile data and eliminate spurious effects caused by nonzero terms at the end points of the profile data set.

With one exception, all samples used in this study were isotropic, and consequently the $\mathrm{PSD}(f_x, f_y)$ function had polar symmetry. For these surfaces, we used a simplified 2-D isotropic form of the PSD obtained by first changing from Cartesian coordinates to polar coordinates:

$$f = (f_x^2 + f_y^2)^{1/2},$$
$$\theta = \tan^{-1}\left(\frac{f_y}{f_x}\right). \quad (3)$$

Then we averaged the resulting $\mathrm{PSD}(f, \theta)$ over the azimuthal angle to yield the 2-D isotropic PSD:

$$\mathrm{PSD}_{2\text{-D}}(f) = \frac{1}{2\pi} \int_0^{2\pi} \mathrm{PSD}(f, \theta)\mathrm{d}\theta. \quad (4)$$

The averaging had a further advantage. In general, the measured PSD is not completely symmetric because of measurement errors and also because the section of surface being measured might not be a good statistical representation of the whole surface. However, because we have the additional knowledge that the surface is actually isotropic, the averaging over all angles helps to reduce the measurement errors.

Each instrument that measured a surface profile or area topography included a certain range of surface spatial frequencies. Also, we measured several places on a surface using the same conditions. In addition, different profile lengths or areas could be chosen for measurements with the same instrument. All the different PSDs could then be combined provided that two conditions are fulfilled: (1) The spatial frequency ranges corresponding to the different measurements should at least partially overlap. This condition is easily met by selection of appropriate image sizes and sampling distances. (2) In the overlapping regions, the different PSD functions should not differ significantly. To meet this condi-