Extended-Range AFM Imaging for Applications to Reflectance Modeling

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Abstract
A technique employing a 3D morphological image-registration algorithm is demonstrated for stitching together high-resolution surface images obtained with a commercial atomic-force microscope (AFM), producing 3D surface images up to 1mm long with lateral resolution ~ 100nm. These images can be applied to reflectance modeling by extracting surface parameters to be used as inputs for reflectance models, for instance the previously-published Coherence Model [BG. Hoover and VL. Gamiz, J. Opt. Soc. Am. A 23, 314 (2006)], which utilizes the surface roughness and autocorrelation derivatives in the large-roughness approximation. Surface moments estimated from extended-range AFM images demonstrate lower uncertainty at all frequencies and substantial reduction of sampling artifacts at low frequencies, enabling improved estimates of surface parameters. The autocorrelation of a nearly monoscale diffuse-gold surface is measured out to 800μm separation, and the autocorrelation of a multiscale tin surface provides parameters that verify the Coherence Model fit to the measured quasimonostatic BRDF.

1 Introduction
Surface reflectance modeling is a key capability for accurate and efficient simulation and analysis of radiometric observables, with pressing applications in machine-vision, laser safety, and laser-manufacturing, among many others. Physical reflectance models are based on measurable surface parameters at scales down to at least the illumination wavelength. Such parameters have been conventionally measured with stylus profilometers [1]-[2], although these cannot easily obtain sub-micron resolution or accurate measurements of many surfaces that are actually scratched by the stylus tip [3]. Atomic-force microscopy (AFM), with probe forces in the nN range and standard resolutions in the nm range, is better suited to obtain parameters on a practical range of surfaces,
but is typically limited to an image field-of-view (FOV) under 100\(\mu m\) on a side corresponding to range limitations of piezoelectric probe actuators. The limited size of the AFM FOV implies undersampling of low-frequency surface features, which can corrupt estimates of surface parameters derived from AFM images.

AFM data has been applied to verify reflectance models of surfaces that satisfy limiting approximations [4], for instance monoscale roughness larger than the illumination wavelength [5]-[6], for which only high-frequency surface features affect the reflectance function or bidirectional reflectance distribution function (BRDF) for laser scattering (see Section 3.1). It is also desirable to apply AFM data to smoother surfaces for which low frequencies become important. Furthermore, most real-world surfaces contain multiscale or composite roughness [7], for which low-frequency features corrupt parameter estimates even in the large-roughness approximation. Extended-range AFM (ER-AFM) benefits reflectance modeling in all of these cases.

2 Extended-Range Atomic-Force Microscopy

Previously published extended-range AFM imagery is surveyed in Table 1 [8]-[12]. Only published imagery is cited; other industrial systems are known to be in use and possibly protected as trade secrets. Most extended-range AFMs are dual-stage systems wherein a conventional AFM head or the sample is mounted on a long-range stage under closed-loop control. While dual-stage systems can be relatively fast, they typically have different resolutions in the orthogonal lateral directions and require painstaking care to ensure the accuracy of the long-range stage [13]. As a result, dual-stage systems appear prohibitively expensive for all but large industrial applications.

<table>
<thead>
<tr>
<th>Parameter → System</th>
<th>Type</th>
<th>Lateral Resolution (nm)</th>
<th>Max Size (Mpix) ((\mu m \times \mu m))</th>
<th>Acquisition Time (min)</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>LNE (France)</td>
<td>Dual-stage</td>
<td>25</td>
<td>1.45 1000 \times 0.75</td>
<td>25</td>
<td>Sinno (2007)</td>
</tr>
<tr>
<td>PTB (Germany)</td>
<td>Dual-stage</td>
<td>10 \times 1250</td>
<td>0.8 1000 \times 10</td>
<td>13.3</td>
<td>Dai (2012)</td>
</tr>
<tr>
<td>SKL PMTI (China)</td>
<td>Dual-stage</td>
<td>15</td>
<td>1D 7200 (1D)</td>
<td>120</td>
<td>Guo (2012)</td>
</tr>
<tr>
<td>Nanosurf Nanite (Switzerland)</td>
<td>Stitching</td>
<td>400</td>
<td>2 560 \times 570</td>
<td>360</td>
<td>AN00410</td>
</tr>
<tr>
<td>ER-AFM</td>
<td>Stitching</td>
<td>78</td>
<td>15 1170 \times 80</td>
<td>1000</td>
<td>Here</td>
</tr>
</tbody>
</table>

Table 1. Brief survey of published extended-range AFM imagery.

Stitching is an attractive option when speed is not a major requirement. Stitching offers the advantages of maintaining AFM resolution in all dimensions
and employing relatively low-cost commercial hardware. Custom AFM control
and stitching software can be accelerated by faster algorithms and processors. The custom stitching software demonstrated in this paper (stitchAFM, pro-
grammed in Matlab) uses a three-dimensional key-point morphological image-
registration algorithm applied to overlapping high-resolution images obtained
by a standard commercial AFM, with the sample manually translated between
individual images on a standard translation stage. The imagery in this paper
was produced by applying stitchAFM to standard images from the Quesant
Q-Scope 250 AFM at the Air Force Research Laboratory, Kirtland AFB, NM.
The standard images, typically 80μm × 80μm FOV, were acquired in tapping
mode with various probes. The open-loop control and piezoelectric-tube actua-
tor of this late-model AFM necessitate morphological image-registration and
preprocessing to remove streak, wave, and dish artifacts. The open-source util-
ity Gwyddion was used for preprocessing standard images and visualization of
resulting ER-AFM images. Figure 1 is an ER-AFM image of a calibration
grating (Mikromasch TGZ02) taken from a 710μm strip image. The grating aspect
ratio R/A = .033 is enhanced in Fig. 1, while dust and other surface imperfections are hidden by flipping the image over to view the bottom of the grating.

Figure 1. Extended-range AFM image of a calibration grating at two
magnifications, taken from a 710μm strip image with 78nm lateral resolution
(9.3Mpix).

The rough surfaces imaged with ER-AFM to date include the diffuse gold
(Epner) and machine-stock tin coupons pictured in Fig. 2. The gold sample was
originally fabricated as a ladar calibration target [14] and later used to verify
the Coherence Model against surface parameters extracted from standard AFM
imagery [5]-[6]. Both of these surfaces have large roughness relative to visible
and NIR wavelengths, and both have high-frequency features inaccessible to
stylus profilometers. The diffuse-gold surface is nearly monoscale with minor very-low-frequency features (because its substrate is not optically flat), while the tin surface is riddled with low-frequency features including striations, pits, and scratches.

Figure 2. Diffuse gold (left) and tin samples measured by ER-AFM.

As previously shown, the surface parameters estimated from standard AFM images of the diffuse-gold surface enable verification of the Coherence-Model fit to the NIR quasimonostatic BRDF [5]-[6]. Under the large-roughness approximation only the roughness and autocorrelation derivatives near the origin are needed [15]. The autocorrelation of this surface estimated from standard AFM images is however not accurate for larger separations; specifically it does not go to zero for large separations, implying that its applicability for reflectance modeling is limited to the large-roughness approximation. The surface autocorrelation estimated from standard AFM imagery is, for instance, not accurate enough to apply to longer wavelengths for which the large-roughness approximation does not hold. Many non-optical applications also require an accurate autocorrelation out to large separations. Figures 3-4 show how ER-AFM overcomes this limitation.

Figure 3. Autocovariance of diffuse-gold surface estimated from 62μm-wide ER-AFM strip images 80μm, 240μm, 480μm, and 827μm long.

The autocovariance of the diffuse-gold surface estimated from ER-AFM images of different lengths is shown in Fig. 3. While the shape of the moment near the origin remains nearly constant, larger images result in lower uncertainty at all frequencies and substantial reduction of sampling artifacts at low
frequencies [16]. The error bars represent the standard deviations of the moment over the short dimension at each separation argument. Significantly, the moment estimate from the longest ER-AFM image goes to zero monotonically, behavior which is shown in Fig. 4 to hold to within 10\% for separations out to 240\mu m and to within 20\% for separations out to 800\mu m. The fluctuations about zero in Fig. 4 could be due to artifacts in the individual frames of the open-loop piezo-tube AFM and/or a non-optically-flat substrate. Improving these results with a decoupled closed-loop AFM and flat substrate is a goal of future ER-AFM development.

Figure 4. Long-range autocovariance of diffuse-gold surface estimated from 1170\mu m-long ER-AFM strip image.

The roughness extracted from large ER-AFM images is larger than that extracted from standard AFM images used for previous Coherence-Model verifications [5]-[6] because larger images pick-up low-frequency components, likely substrate non-planarity for the diffuse gold. The diffuse-gold roughness estimated from standard AFM images and used for previous verifications is \( \sigma_{\text{high}} \approx 800\text{nm} \) [6], while the roughness estimated from the 1170\mu m-long strip image is around 1100nm, implying \( \sigma_{\text{low}} \approx 300\text{nm} \). In this case the low-frequency component is unlikely to affect the reflectance at any wavelength, but, as implied in Section 3.1, if \( \sigma_{\text{low}} > \sigma_{\text{high}} \), then the low-frequency component could become relevant at longer wavelengths where the high-frequency roughness no longer limits the coherence of the scattered surface field. ER-AFM therefore provides a means to study and potentially define a frequency-dependent roughness \( \sigma_h(\lambda) \) critical to the description of broadband reflectance from multiscale surfaces.

3 Reflectance Modeling

3.1 BRDF of a Multiscale Surface

A multiscale or composite surface is defined as a surface with height variations expressible as the sum of two or more random processes with widely different moments. Most common surfaces are multiscale with the surface of the ocean on
a windy day a familiar example. This section gives a brief theoretical description in terms of the Coherence Model to help explain the results of the next section. While the Coherence Model differs fundamentally from the Kirchhoff scattering model [5], the following results for multiscale surfaces are essentially the same as those stated by Beckmann a half-century ago based on the Kirchhoff model [7].

Two surfaces are defined by their height functions \( h_1(x) \) and \( h_2(x) \), which are real-valued independent random processes and are both zero-mean. The multiscale surface is \( h(x) = h_1(x) + h_2(x) \), which is also zero-mean. The surface autocorrelation function is

\[
R_{h}(\Delta x) = \langle h(x) h(x + \Delta x) \rangle = \langle (h_1(x) + h_2(x)) (h_1(x + \Delta x) + h_2(x + \Delta x)) \rangle = R_1(\Delta x) + R_2(\Delta x),
\]

(1)
since the cross-correlations are zero. The variance is the autocorrelation evaluated at zero, ie

\[
R_{h}(0) = \langle h^2(x) \rangle = \sigma_{h_1}^2, \tag{2}
\]

it is easy to show that \( \sigma_{h}^2 = \sigma_{h_1}^2 + \sigma_{h_2}^2 \) for the composite surface. The Coherence Model considers the surface to be a phase screen from which only single-scattering occurs without shadowing. Under these conditions, if \( h(x) \) is Gaussian distributed with arbitrary \( R_{h}(x) \), the scalar coherence function of the scattered quasimonochromatic optical field of center wavelength \( \lambda \) is proportional to

\[
\gamma(\Delta x) \propto \exp \left[ -\frac{4\pi^2}{\lambda^2} (1 + \cos \theta_i)^2 (\sigma_{h}^2 - R_{h}(\Delta x)) \right], \tag{3}
\]

where \( \theta_i \) is the angle of incidence to the average surface. At normal incidence this becomes

\[
\gamma(\Delta x) \propto \exp \left[ -\frac{16\pi^2}{\lambda^2} (\sigma_{h}^2 - R_{h}(\Delta x)) \right]. \tag{4}
\]

The BRDF is then the Fourier transform of the coherence function per the van Cittert-Zernike theorem [15]. This expression implies that, no matter how rough the surface (as quantified by \( \sigma_{h}^2 \)), if the surface height varies slowly, such that \( R_{h}(\Delta x) \approx R_{h}(0) \), over lateral distances that are large compared to the wavelength, then the BRDF will be narrow. This describes low-frequency roughness components of many common surfaces.

For the composite surface it is easy to show that

\[
\gamma(\Delta x) \propto \exp \left[ -\frac{16\pi^2}{\lambda^2} (\sigma_{h_1}^2 - R_{h_1}(\Delta x)) \right] \exp \left[ -\frac{16\pi^2}{\lambda^2} (\sigma_{h_2}^2 - R_{h_2}(\Delta x)) \right]. \tag{5}
\]

The BRDF of the composite surface is therefore the convolution of the BRDFs of the individual surfaces. If a high-frequency roughness component \( h_1(x) \)

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rides atop a large-scale, low-frequency roughness component \( h_2(x) \), then the high-frequency component will determine the BRDF provided \( 16\pi^2\sigma_1^2 \gg \lambda^2 \); the BRDF of the composite surface will be approximately the BRDF of the high-frequency component, slightly broadened by the effect of the low-frequency component. This condition prevails for the diffuse metals considered in this paper. This also assumes the illuminated area is much larger than the correlation area of the low-frequency component. If it is not, then the Coherence Model is not directly applicable to reflection from the low-frequency component, which can instead be described by aberration theory. Alternatively, as demonstrated in Section 3.2, the illuminated area can be small enough and strategically located to avoid low-frequency features beyond 1st-order tilt.

### 3.2 Coherence Model of Diffuse Tin

Figure 5 is an ER-AFM image of the rough tin sample pictured in Fig. 2, taken from a 970\( \mu \)m-long strip image. Low-frequency features, like the scratch apparent on the left side of Fig. 5, corrupt estimates of surface parameters from standard AFM images. Table 2 indicates the convergence of parameter estimates for this surface as the ER-AFM FOV increases. \( \rho_i \) is the \( i \)th radial derivative of the surface autocorrelation function evaluated near the origin [15]. The Coherence Model provides a nearly closed-form BRDF solution by assuming a quadratic series expansion of the surface autocorrelation. In the large-roughness approximation, specifically when \( 16\pi^2\sigma_1^2 \gg \lambda^2 \) as derived above, this is a Taylor series that is more accurate when \( \rho_3 \) and higher derivatives are comparatively small.

![Figure 5](image.png)

**Figure 5.** Image of diffuse tin surface taken from a 970\( \mu \)m-long ER-AFM strip image with 156nm lateral resolution.

<table>
<thead>
<tr>
<th>( L (\mu \text{m}) )</th>
<th>( \sigma_3 (\mu \text{m}) )</th>
<th>( \rho_1 (\mu \text{m}^{-1}) )</th>
<th>( \rho_2 (\mu \text{m}^{-3}) )</th>
<th>( \rho_3 (\mu \text{m}^{-5}) )</th>
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<tr>
<td>80</td>
<td>0.105</td>
<td>-0.065</td>
<td>-0.230</td>
<td>0.190</td>
</tr>
<tr>
<td>200</td>
<td>0.226</td>
<td>-0.019</td>
<td>-0.0007</td>
<td>-0.0007</td>
</tr>
<tr>
<td>500</td>
<td>0.454</td>
<td>-0.0043</td>
<td>-0.0005</td>
<td>0.0000</td>
</tr>
<tr>
<td>700</td>
<td>0.464</td>
<td>-0.0046</td>
<td>-0.0002</td>
<td>0.0000</td>
</tr>
</tbody>
</table>

**Table 2.** Parameters of diffuse tin surface estimated from \( L\mu \text{m} \times 57\mu \text{m} \) ER-AFM images.
Figure 6(a) is a photo of the bistatic BRDF of the diffuse tin for $\lambda = 633nm$ illumination, 2mm $\odot$ probe spot, and near-normal AOI. The quasimonostatic version of this BRDF (scanning the sample rather than the receiver) measured with a receiver solid angle of $\Omega_R = .17msr$ and 0.4° angular step is indicated by the points in Fig. 6(b). Verification is achieved by fitting the measured BRDF with the Coherence Model using only surface parameters from Table 2. Parameters estimated from the standard AFM image ($L = 80\mu m$) yield a very poor fit, with an overly diffuse model solution despite underestimation of the roughness. Without ER-AFM the modeling effort would end there. But larger image FOVs improve the parameter estimates such that the parameters highlighted in Table 2 produce the fit shown in Fig. 6(b). The Cauchy-like BRDF implies a microtexture with sharp edges [15]. Local optimization of the parameters about the raw ER-AFM estimates, which would certainly improve the fit, was not performed in order to demonstrate the raw capability of the technique. As noted for the diffuse-gold in Section 2, the roughness estimate from the largest ER-AFM image is too large, again because larger images encompass low-frequency features, like the scratch in Fig. 5, that do not affect the BRDF when high-frequency roughness is dominant as specified in Section 3.1. This is also consistent with the BRDF measurement, for which the small probe spot was located to illuminate an area that produced the relatively unaberrated reflectance distribution seen in Figure 6.

![Figure 6](image)

Figure 6. Quasimonostatic BRDF of diffuse tin at $\lambda = 633nm$: (a) Irradiance on aperture stop, with the probe beam passing through the eyelet. (b) Measured normalized cosine-corrected BRDF and unoptimized Coherence Model fit from ER-AFM surface parameters.

## 4 Conclusions & Acknowledgments

AFM is a valuable tool for reflectance modeling, and extended-range AFM (ER-AFM) is essential for modeling common multiscale surfaces. Stitching is a cost-effective approach to ER-AFM that is currently slow but can be accelerated...
with faster algorithms and processors. Here ER-AFM is shown to improve estimates of surface parameters, which are input to the Coherence Model to verify fits to BRDFs of diffuse-metal reflectors. Other reflectance models can be used. Once a model is verified for a particular class of reflectors, it may eventually be possible to replace costly radiometric measurements with ER-AFM measurements for general radiometric simulations and analyses.

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References


[16] The autocovariance is the autocorrelation of a non-zero-mean process, which is simply a computational detail in the current context. The autocorrelation is the Fourier transform of the power spectral density (PSD), so small autocorrelation arguments correspond to high-frequency surface features and vice versa.