Surface Roughness of Thin Films

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Abstract

We have calculated corrections to the Fresnel coefficients based on surface roughness from a perfect conductor. These corrections are important to accurately determine the index of refraction data from reflectance measurements at extreme ultraviolet wavelengths. The corrections are based on two-dimensional scattering calculations of arbitrary precision with s-polarized light from a perfectly conducting surface of 200 wavelengths in width. The calculations are valid for large surface roughness heights and near-grazing angles, conditions where approximations in previously published approaches breakdown. The calculations show a general agreement with Debye-Waller form, but show evidence of a significant correction needed to that form as well.

1 Background

Good reflective optics for extreme ultraviolet (EUV) wavelengths are becoming increasingly important. They have found important applications in astrophysical observations[1, 2], smaller computer chips, improved microscopes, and plasma diagnostics, for instance[3]. Effectively designing these optics requires a good knowledge of the index of refraction of a variety of optical materials in these wavelength regions[4].

Unfortunately, the data on the optical properties of materials in this wavelength region are of lower quality and are more scarce than at visible and ultraviolet wavelengths. The BYU Thin Films Group has undertaken a project to determine optical constants of a variety of elements and compounds at EUV wavelengths which show promise for use in reflective optics[5, 6, 7, 8, 9]. The index of refraction of these materials is derived from reflection and transmission data on thin films.

The theory for the reflectance of light from thin films is well known assuming the films have abrupt planar interfaces[10, 11, 12]. Interfacial roughness and gradients in the index of refraction at the interfaces require corrections to these formulas. A set of commonly used corrections are the Debye-Waller correction[13] and an improvement by Nevot and Croce[14, 15]. The Debye-Waller correction involves multiplying the Fresnel coefficients at each interface by a factor

$$e^{-2q^2\sigma^2} \,, \tag{1}$$

where σ is the rms height of the gaussian roughness on the surface. The variable q is the transverse momentum transfer given by

$$q = \frac{2\pi n}{\lambda} \sin\theta \,, \tag{2}$$

where λ is the vacuum wavelength, n is the index of refraction, and θ is the incident angle measured from grazing. The Nevot-Croce correction uses an average momentum transfer from each side of the interface, giving a correction factor of

$$e^{-q_1 q_2 \sigma^2} \,. \tag{3}$$

These approximations suppose a gaussian variation in surface height at all spatial frequencies and ignore effects of near field interactions between different areas of the surface. Nonetheless, they provide a good first-order roughness correction under some conditions[16]. Stearns has improved on these calculations, but his work is under the assumption that there are low reflectances at each angle and that the roughness height is small compared to a wavelength[18].

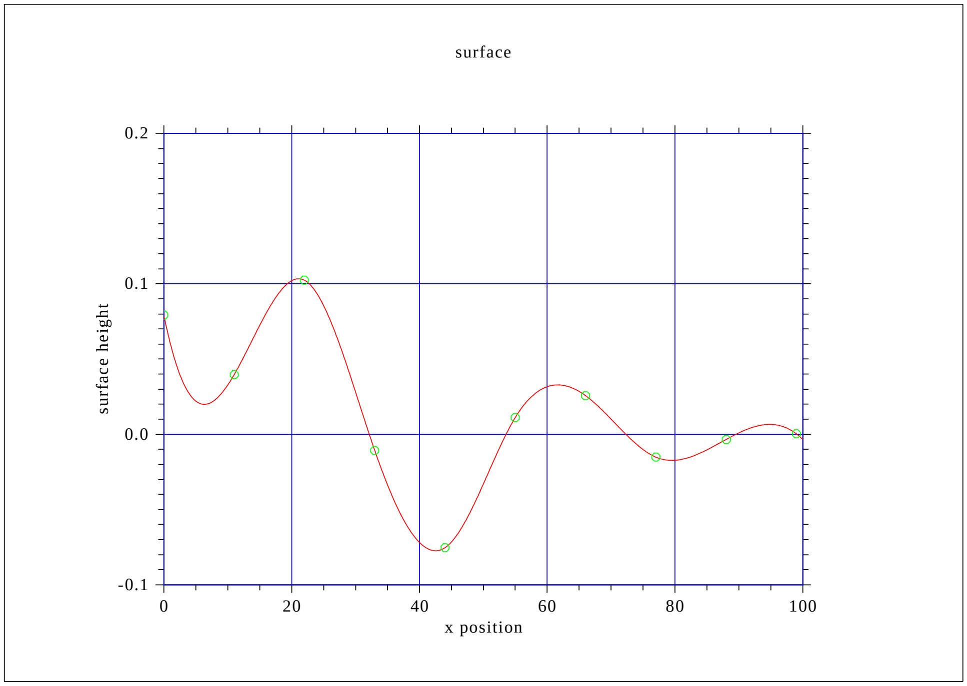

Figure 1: Example surface with an rms height of 0.06 wavelengths and a knot spacing of 11 wavelengths.

2 Approach

In order to accurately determine the index of refraction in EUV thin films, it is sometimes important to be able to account for the surface roughness better than the approximations developed by previous authors. To do this, we computed the scattering from a 200 wavelength long plate in two dimensions with a random surface having controlled roughness. The reflected light was computed to arbitrary precision using the algorithms developed by Johnson[19]. These algorithms were too slow for this application as written in Matlab, but were rewritten in FORTRAN and run on marylou4, a supercomputer cluster at Brigham Young University consisting of 1260 dual core Intel EM64T running at 2.6 GHz in a reasonable amount of time.

The scattering was computed for random planar surfaces with added rms roughness of heights between 0.01 and 0.1 wavelengths. Rather than use a gaussian surface with all possible spatial frequencies, we computed the roughness height at equally spaced points between 0.5 wavelength and 20 wavelengths. The surface between those points was approximated with a cubic spline using the points as knots. This gave us a good model of the kinds of physical surfaces we expected to see in our samples.

Figure 1 is a plot of an example surface with an rms roughness of 0.06 wavelengths and a knot spacing of 11 wavelengths. The green circles are the locations of the knots and the red line represents the surface itself. Figure 2 is another sample surface, this time with an rms roughness of 0.04 wavelengths and a knot spacing of 5 wavelengths. Notice how the closer knot spacing results in higher spatial frequency components. As a final extreme example, Figure 3 is a plot of a sample surface with an rms roughness of 0.1 wavelengths and a knot spacing of 1 wavelength.

The roughness correction for a perfect conductor is the absolute value of the ratio of the far field for a rough surface to that of a smooth surface. We tried several different approaches for computing this ratio. The first challenge we faced was that our surfaces showed significant broadening of the reflection peak and had significant side-lobes due to diffraction. Figure 4 is the far field intensity of the reflection from a smooth surface 200 wavelengths in width. The diffraction is an artifact of limiting our surface to the relatively small size of 200 wavelengths.

We tried three approaches to comparing the reflected beams from the smooth and rough surfaces:

1. We compared the areas under the central peaks. Since these peaks are artificially broadened, all of the light in the central peak should make it into the detector. This was straightforward for smooth

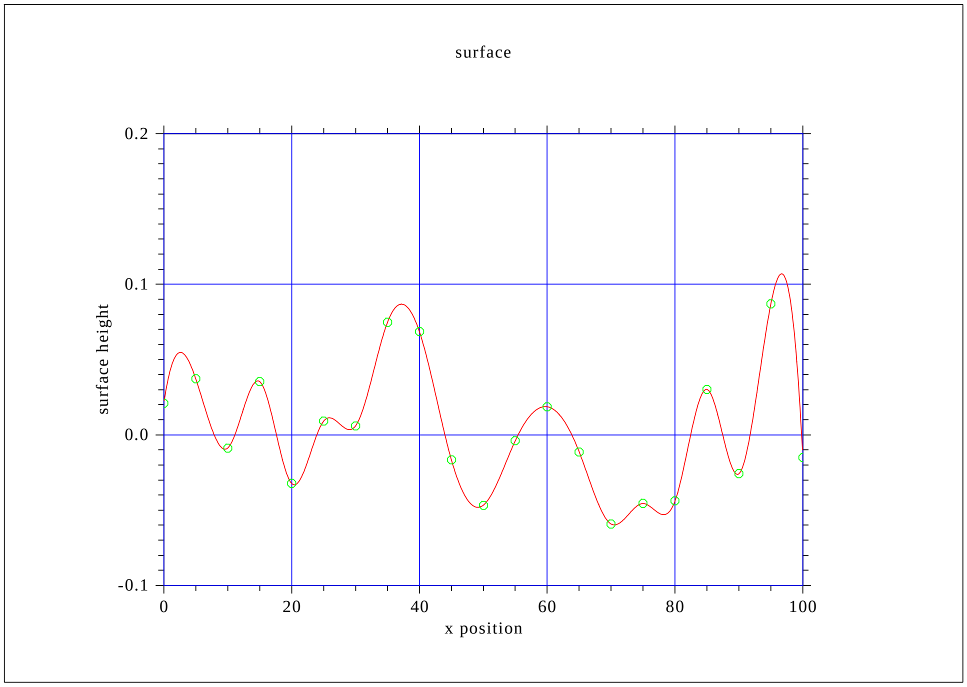

Figure 2: Example surface with an rms roughness of 0.04 wavelengths and a knot spacing of 5 wavelengths.

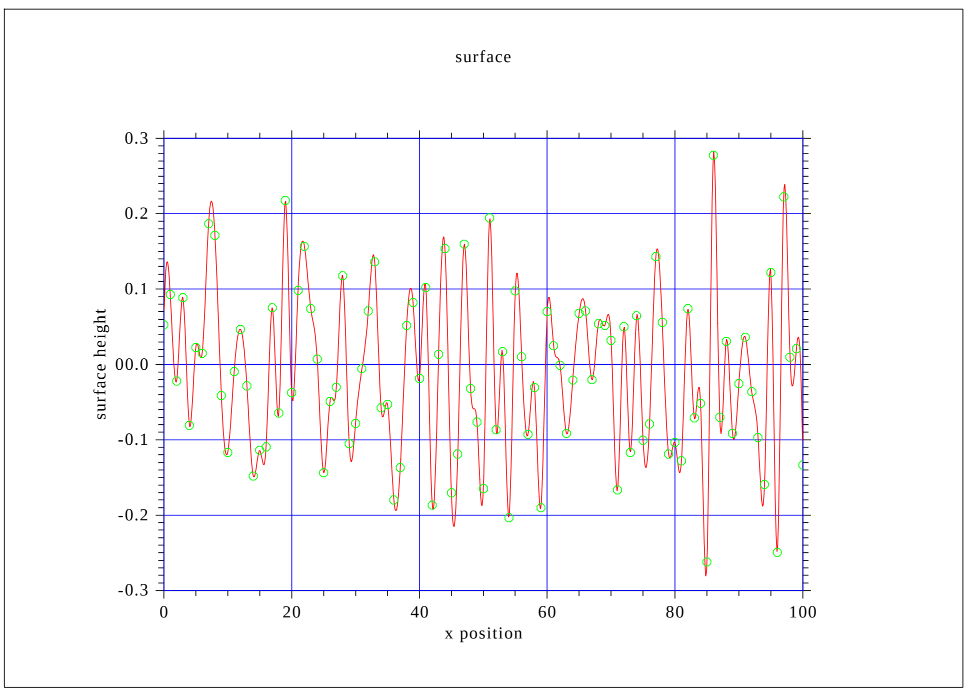

Figure 3: A sample surface with an rms roughness of 0.1 wavelengths and a knot spacing of 1 wavelength.

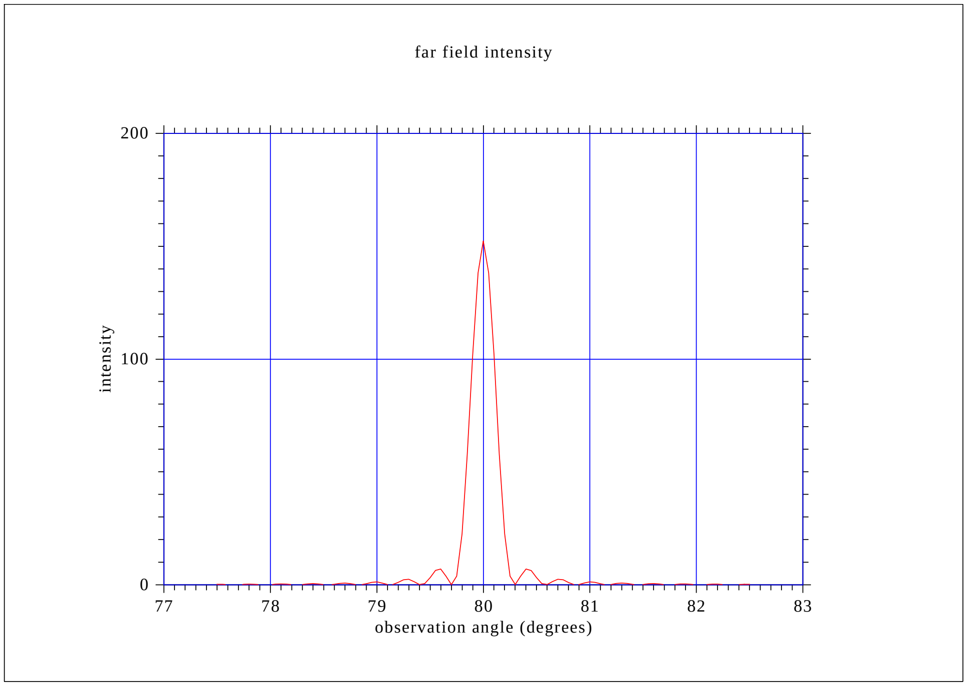

Figure 4: Reflected intensity from a smooth surface 200 wavelengths wide.

surfaces, but caused problems with rough surfaces where the diffuse scattering overlapped with the central peak. Figure 5 is a plot of the far field intensity after scattering a plane wave from the same surface as in Figure 4 but with roughness with $h = 0.1$ wavelengths added. Note the difficulty in distinguishing the diffraction peaks from the scattering due to roughness.

2. We integrated the light over an angular range matching my estimate of the angular acceptance of our detector we use at BYU and at the Advanced Light Source at Berkeley. This seemed like a reasonable match to our experimental conditions. Unfortunately, it suffered from some of the same problems as the first approach. It also made the results very experiment-specific.

3. Lastly, we compared with heights of the central peaks. This was a simple calculation and seemed to be at least as reliable as the other methods. It also was the most reproducible between runs and was independent of the solid angle of the detector. We used this approach for the subsequent analysis.

These calculations are very lengthy, taking hours of supercomputer time on many processors. Because of this, we set about to find efficient semi-empirical formulas for the reflectance correction as a function of the knot spacing, the incident angle and the rms roughness. We plan to use these in our fitting programs to more accurately determine the index of refraction of our samples at EUV wavelengths.

3 Results

The Debye-Waller formula in Equation 1 suggests that the reflectance might be a function of the log of a polynomial. To check this ansatz, we plotted $-\ln(R)$ as a function of qh for each set of knot spacings we used, where h is the rms roughness of the surface. The ansatz turned out to be an even better guess than we anticipated. Figure 6 is a plot of the negative log of the reflectance as a function of qh for knots spaced three wavelengths apart. The error bars represent the spread of the reflectance in an average over 100 random surfaces. (The error in the plotted means would be about a factor of 10 smaller than this.) Note how the points, which come from different combinations of θ and h, tend to lie on a single curve. This was typical of all our curves, greatly reducing the number of parameter combinations needed to characterize the roughness correction.

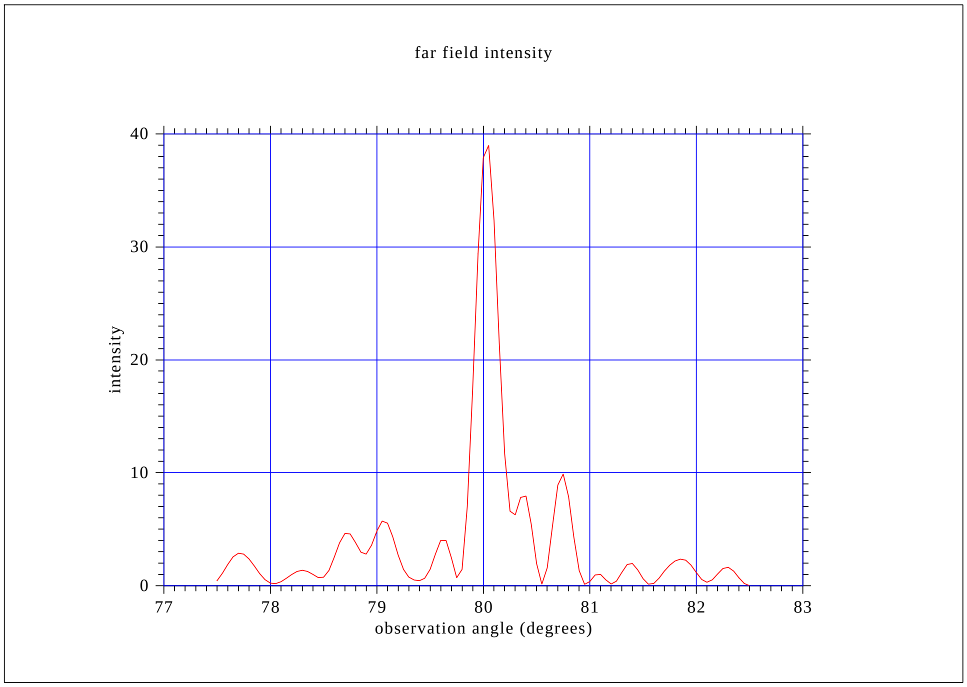

Figure 5: Far field intensity after scattering a plane wave from a rough surface with rms roughness of 0.1 wavelengths and width of 200 wavelengths.

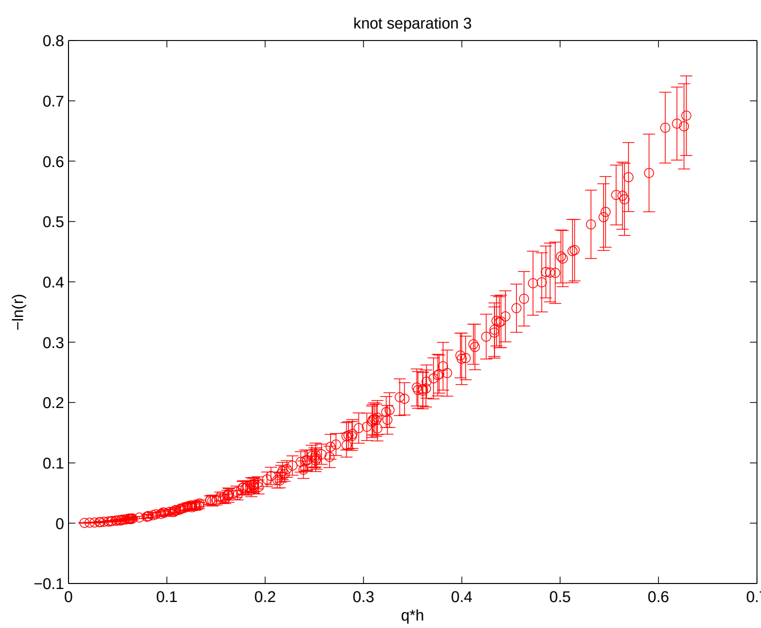

Figure 6: Functional dependence of the negative log of the reflectance on the parameter qh for a mirror with spline knots three wavelengths apart.

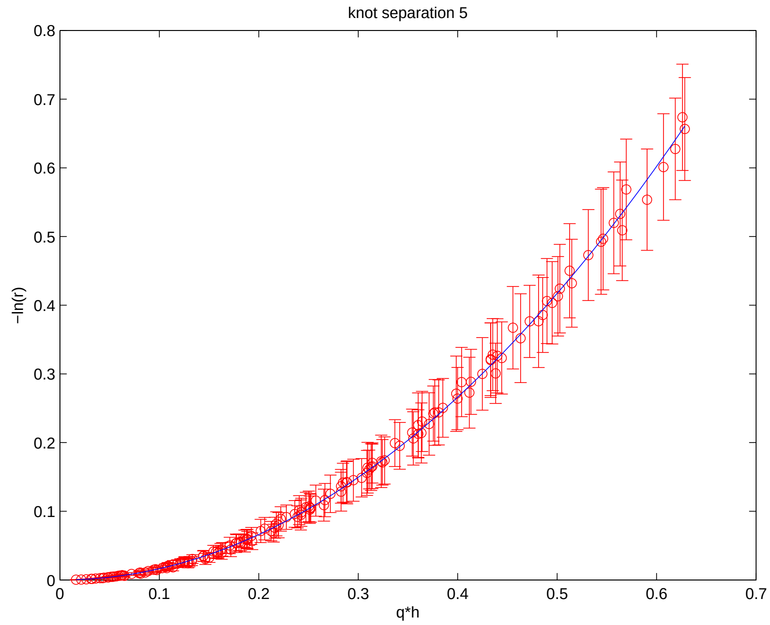

Figure 7: Cubic polynomial fit (blue curve) to the combined qh data for a knot separation of 5.0 wavelengths.

With this observation, we proceeded to fit each of the curves for various knot separations to cubic polynomials in qh with the constant terms set equal to 0. The constant term should be identically zero, since $qh = 0$ corresponds to no roughness and reflectance of 1 by definition. Figure 7 is an example of a fairly good fit for a knot spacing of 5.0 wavelengths. Figure 8 is an example of a poorer fit for a knot spacing of 17.0 wavelengths.

We then took the polynomial fit coefficient for each knot separation and create three graphs of the linear (Figure 9), quadratic (Figure 10), and cubic (Figure 11) fit coefficients.

There is some inconsistency between the points in the various plots. Further analysis of the data is needed to understand why many points seem to follow a definite pattern, but a few look much different than the others. The higher order coefficients seem to deviate from the relatively smooth curve I would expect by more than their error bars.

4 Conclusions

The goal in this project is to come up with a general set of functions that can be used to predict the roughness correction as a general function of q from Equation 2 and the knot separation f. From the graphs in Section 3, it looks like a complete solution to that question is still premature. However, the following conclusions can be drawn.

1. The linear component of the f dependence is consistent with 0. Only quadratic and cubic terms should be used in the fit.

2. The quadratic component of the f dependence has a constant term which is between about 1.4 and 1.7. The rest of the dependence on f needs to be studied further. The significance and magnitude of this term are roughly consistent with what one would expect from Equations 1 and 3.

3. The cubic term looks like it has a constant in its f dependence of about 0.25 and a linear term between about -0.02 to -0.05. It is probably significant. This means that using just the Debye-Waller or Nevot-Croce corrections for roughness are insufficient under some conditions.

We are continuing to generate more data in order to improve our statistics and the quality of the polynomial fits. With this additional data, it should be possible to give a definite set of semi-empirical rules for computing

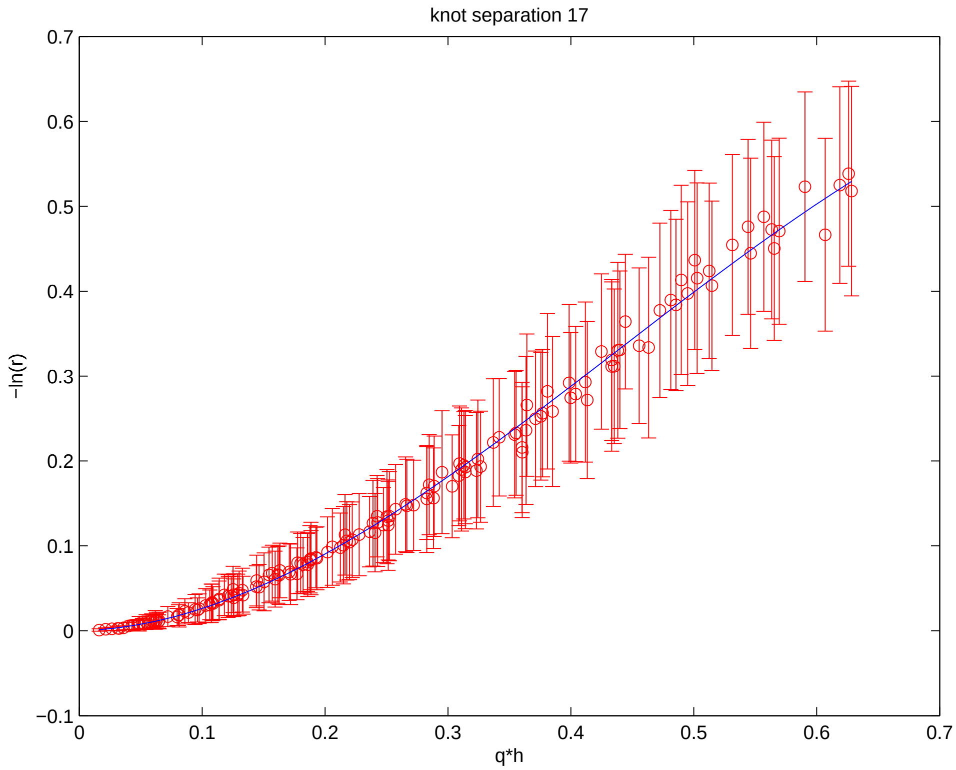

Figure 8: Cubic polynomial fit (blue curve) to the combined qh data for a knot separation of 17wavelengths.

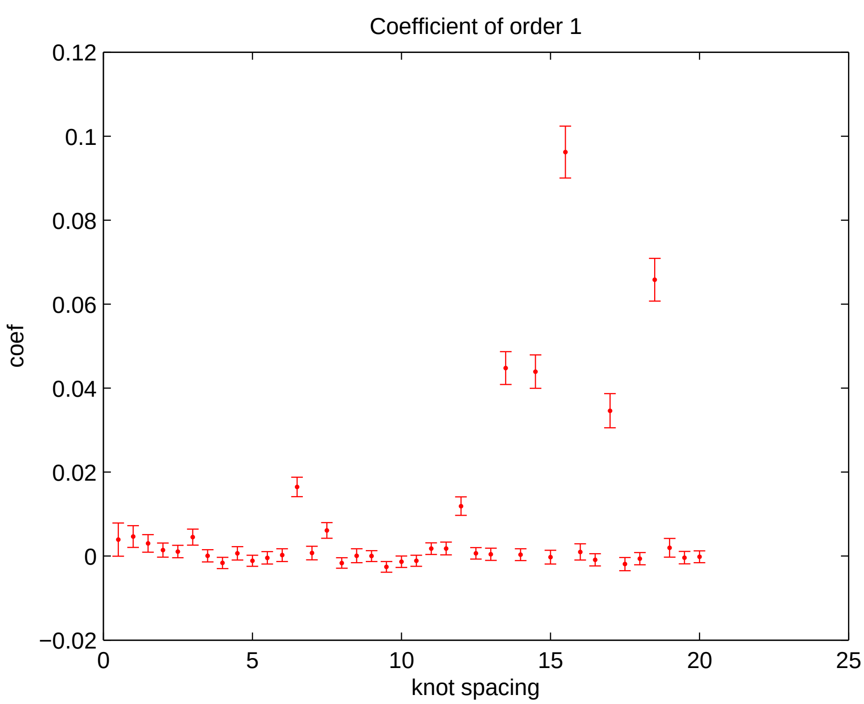

Figure 9: Linear coefficients in cubic fits of $-\ln r$.

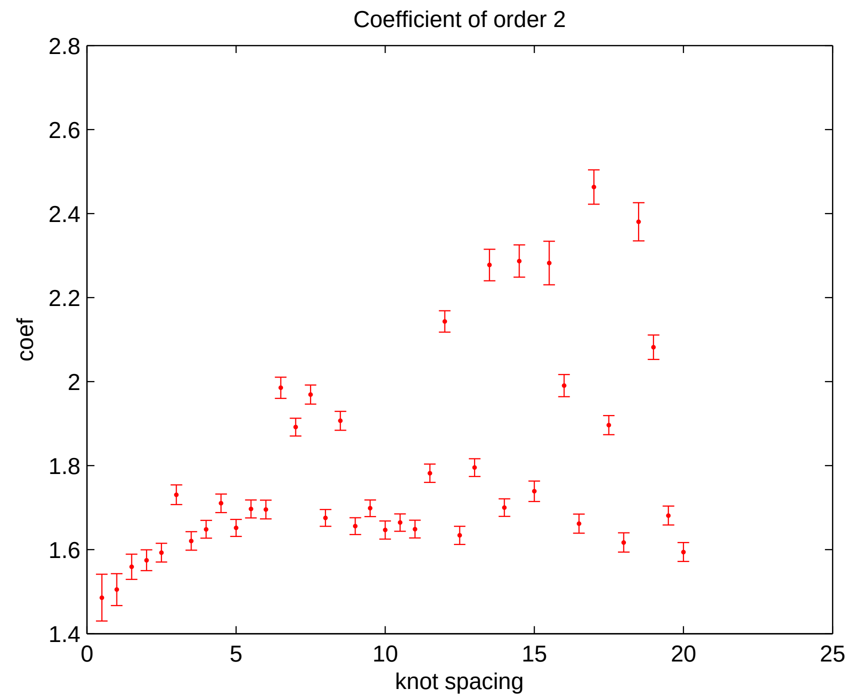

Figure 10: Quadratic coefficients in cubic fits of $-\ln r$.

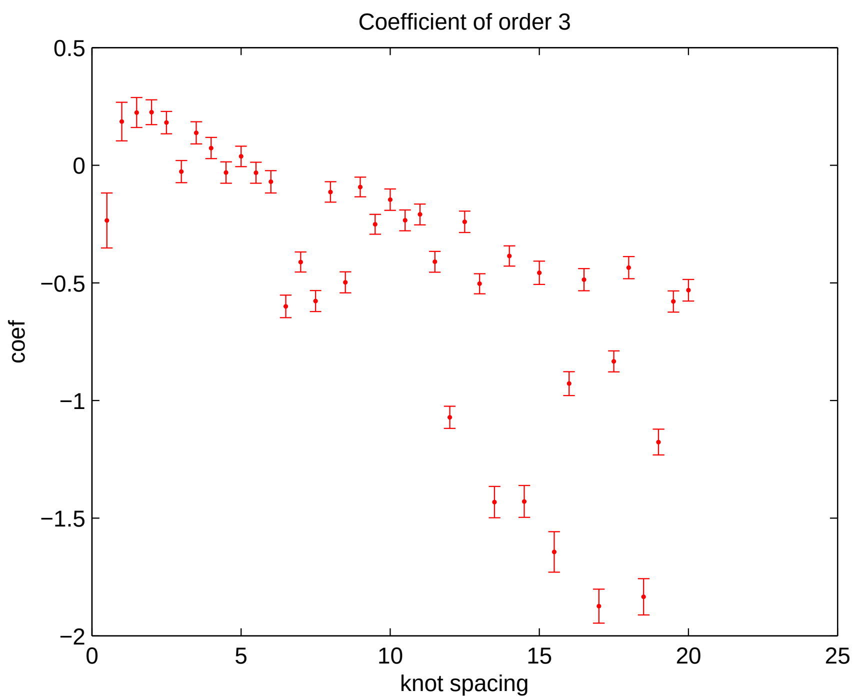

Figure 11: Cubic coefficients in cubic fits of $-\ln r$.

a roughness correction as a function of f and qh. We are also working on replacing the perfectly conducting surface with a dielectric one and studying the difference in these results if we use light with p-polarization instead of s-polarization.

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