Specular gloss simulations of media with small-scale roughness

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We study the effect of microroughness on the simulated specular reflection (i.e., gloss). We use the discrete-dipole approximation and compare the results to the Bennet–Porteus approximation. This study is originally applied to print toners for paper industry, but the results are general and apply to all other surfaces with small-scale roughness.

INTRODUCTION

In paper industry, one important feature in digital printing revealing a good image quality is the print gloss. Roughness of paper, determined on a macroscale, is usually exhibiting a good correlation with gloss[1]. Attempts to correlate microroughness properties with gloss has been presented in several reports (e.g. [2, 3]). Despite several studies, the impact of the toner substrate surface roughness is lacking.

The surface of paper printed with toners consists of close-packed toner particles. Individual toners are quite cylindrical with diameters of about 8 µm and thicknesses of about 2–3 µm. The toner surface can be measured with the atomic force microscope (AFM, in tapping mode). Images obtained with AFM show that the surface standard deviation is typically about 21 nm with AFM image size of 3×3 µm and 31 nm with 10×10 µm. Therefore, the study of the effect of toner surface roughness on specular reflection (gloss) can be generalized to a generic case of surface with roughness in scales smaller than the wavelength.

Suitable methods for analysing the effect of the small-scale roughness on light scattering have been lacking. Recently, computational methods, e.g., the discrete-dipole approximation (DDA; see, e.g., [4]), have become relevant due to the increased resources of modern computing clusters. The accuracy of DDA is fairly good compared to exact wave-optical methods[5], and thus DDA can be used to check the validity of other approximations.

METHODS FOR ANALYZING THE SPECULAR REFLECTION

Reflected light from rough surfaces is a sum of coherent scattering, or specular reflection, and incoherent or diffuse scattering. With a Gaussian rough surface with surface standard deviation σ and correlation length τ, both smaller than the wavelength λ, the specular part can be estimated to some extent with analytical approximations. The exact specular component from a smooth surface can be estimated with the Fresnel reflection coefficient and the effect of surface σ can be added with the Bennet–Porteus (B–P) factor[6]. More detailed approximations include the Muinonen–Smythe–Kirchhoff (MSK) approximation[7] for coherent scattering near the specular direction along the principle plane, and the Beckmann–Kirchhoff (B–K) model[8] for coherent scattering off from the principal plane. The results from comparison with the DDA method show that the abovementioned MSK and

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B–K approximations can be quite good in some cases but, especially with non-zenith incoming light, the results off the principal plane with the B–K approximation are not accurate enough (results not shown here).

The Bennet–Porteus (B–P) approximation for gloss G is

$$\mathrm{G}(\sigma) \propto \exp\left(-(4\,\pi\,\sigma\cos(\theta)/\lambda)^2\right), \tag{1}$$

where σ is the surface standard deviation, θ the incoming angle, and λ the wavelength. The proportionality of G and the B–P factor is such that for perfectly smooth surface the B–P factor is one and the gloss value is given by the normalized Fresnel coefficient of the surface. The B–P approximation is very simple to calculate, and thus it is interesting to study its accuracy.

SIMULATION OF GLOSS

We can model the rough surface of cylindrical slab with random height field. We assume the height field to be Gaussian with Matérn (auto)correlation function. The formula of the Matérn correlation function is

$$\mathrm{C}(d) = (2\sqrt{\kappa}\frac{d}{\tau})^{\kappa}\; K_\kappa(2\sqrt{\kappa}\frac{d}{\tau})\;\left(2^{\kappa-1}\,\Gamma(\kappa)\right)^{-1}, \tag{2}$$

where K_κ is the modified Bessel function of the second kind and Γ is the gamma function. The parameters are τ which is the correlation length and κ which controls the smoothness of the surface. Actually, κ controls up to which order the surface will have continuous derivatives. Special cases of Matérn are when $\kappa \to \infty$ when it approaches the Gaussian correlation function, and $\kappa = 1/2$ when it is equal to the exponential correlation function.

We have used four different values for κ to study the effect of the correlation structure of the surface on gloss, $\kappa = 1/2, 1, 2$, and $\kappa \to \infty$. For the correlation length τ, we have used three values: $\tau = 250$, 500, and 1000 nm. The most interesting surface parameter is the surface σ and its effect on gloss. We used σ values from 0 nm to 40 nm with 10 nm steps in our simulated surfaces. An example of realizations of the modeled rough cylinders are shown in Fig. 1.

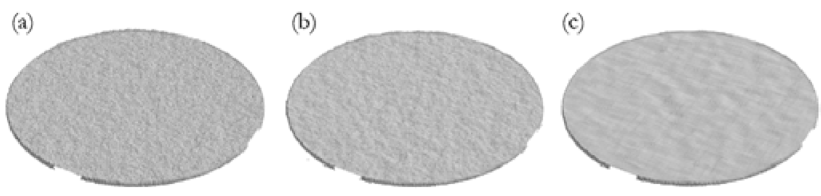

Figure 1. Three realizations of the surface model. All the surfaces have $\tau = 500$ nm and $\sigma = 20$ nm. The leftmost surface has $\kappa = 1/2$ (exponential correlation), the middle $\kappa = 1$, and the rightmost has $\kappa \to \infty$ (Gaussian correlation).

Gloss measurements and DDA

The DDA method produces a map of the reflected intensity from the model surfaces with a given incoming angle. The most interesting part of the reflection in our case is the area around the specular direction. The behavior of the gloss peak can clearly be seen from the

DDA simulation results as in Fig. 2a. However, when comparing the simulated results to the measurements, some data reduction must be done to mimic the measuring configuration, e.g., the TAPPI T 480 standard or similar [9]. In the measurements, the device that captures the reflected flux has some finite acceptance area from where it integrates the flux. With simulated data, we have several options for extracting the gloss value. We can either take the peak value in the exact specular direction or we can integrate over a small area around the specular direction. This integration can be done one-dimensionally (1-D) along the principal plane or, more generally, in two-dimensionally (2-D) on the spherical surface.

The measured gloss values are not the absolute values of the flux, instead the values are compared to the gloss value of the standardized smooth black glass plate [9] with gloss value G of 100 GU (gloss units). If the material refractive index n, especially its imaginary part, that we are interested in is not known, the absolute calibration to black glass is impossible. The relative scale where we standardize the DDA results to the gloss from a smooth cylinder having the same n that we use for the material is sufficient to study the validity of the B–P factor. We found out that all the different methods to extract gloss values (i.e., peak value, 1-D or 2-D integration) will produce about the same outcome when standardized. Therefore, we choose to calculate the 1-D integral along the principal plane with $\pm 4°$ from the specular direction, because its evaluation is more convenient than the 2-D integral. We used $20°$ zenith angle for incoming light.

RESULTS FROM GLOSS ANALYSIS

The surface model with Matérn correlation function C is parameterized with the smoothness parameter κ and correlation length parameter τ. We have used very absorbing material with $n = 1.54 + \mathrm{i}1$ for more prominent surface effects, but we also studied the case $\mathrm{Im}n = 0.015$. The dipole representation of the cylindrical slab has 320 dipoles for the cylinder diameter of 8 µm and 20 dipoles for depth, resulting about 2×10^6 dipoles for the DDA grid, of which about 1.6×10^6 are occupied by the material.

The effect of four different κ's is shown in Fig. 2b. In overall, it seems that the effect of σ in the B–P approximation behaves quite reasonably but overestimates the gloss systematically. The smoothest C, where $\kappa \to \infty$ and the correlation is Gaussian, as in the original derivation of the B–P factor, is closest to the B–P approximation. As the κ has smaller values and the C changes toward the exponential correlation, the difference to the B–P approximation gets larger.

The effect of the correlation length τ is presented in Fig. 2c. All the values of τ give similar shapes to the gloss as a function of σ, but larger τ give more gloss in better agreement with the B–P approximation. This result is in disconjunction with the theoretical basis of the B–P approximation where it is required that $\tau \ll \lambda$, so it seems that this requirement is not that important. If the imaginary part is small, all the surface effects become less pronounced as seen in Fig. 2d.

In conclusion, we note that the B–P approximates quite well the overall shape of the dependence between the small-scale surface deviations and the specular reflection. However, the B–P factor does not take into account the refractive index or the correlation type or length. If more detailed analysis is needed, DDA is a suitable method.

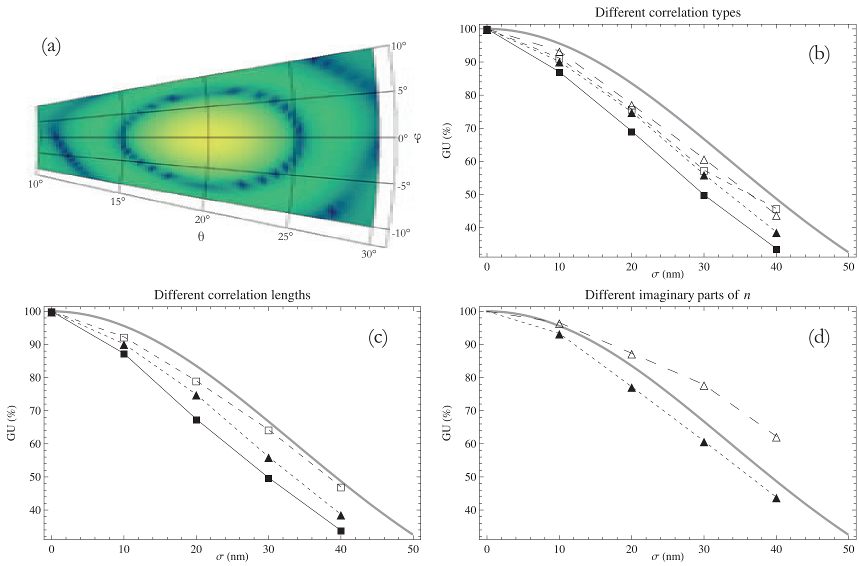

Figure 2. (a) Scattering pattern around the specular direction ($\varphi = 0°, \theta = 20°$) simulated with DDA. Brighter yellow and green areas have higher intensity. (b)–(d) Gloss as a function of surface σ. The gray line shows the B–P approximation. (b) The symbols ■, ▲, □, △ correspond to $\kappa = 1/2, 1, 2$, and $\kappa \to \infty$; $\tau = 500$ nm and $n = 1.54 + \mathrm{i}1$. (c) The symbols ■, ▲, □ correspond to $\tau = 250, 500$ and 1000 nm; $\kappa = 1$ and $n = 1.54 + \mathrm{i}1$. (d) The symbols ▲, △ correspond to $\mathrm{Im}n = 1, 0.015$, $\kappa \to \infty$, $\tau = 500$ nm, and $\mathrm{Re}n = 1.54$.

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