Estimation of gloss from rough surface parameters

Ingve Simonsen\textsuperscript{1}, Åge G. Larsen\textsuperscript{2}, Erik Andreassen\textsuperscript{2}, Espen Ommundsen\textsuperscript{3}, and Katrin Nord-Varhaug\textsuperscript{3}

\textsuperscript{1} Department of physics, NTNU, NO-7491 Trondheim, Norway
\textsuperscript{2} SINTEF Materials and Chemistry, P.O. Box 124 Blindern, NO-0314 Oslo, Norway
\textsuperscript{3} Borealis AS, NO-3960 Stathelle, Norway

Received zzz, revised zzz, accepted zzz
Published online zzz

PACS 42.25.-p,42.70.-a

Gloss is a quantity used in the optical industry to quantify and categorize materials according to how well they scatter light specularly. With the aid of phase perturbation theory, we derive an approximate expression for this quantity for a one-dimensional randomly rough surface. It is demonstrated that gloss depends in an exponential way on two dimensionless quantities that are associated with the surface randomness: the root-mean-square roughness times the perpendicular momentum transfer for the specular direction, and a correlation function dependent factor times a lateral momentum variable associated with the collection angle. Rigorous Monte Carlo simulations are used to access the quality of this approximation, and good agreement is observed over large regions of parameter space.

1 Introduction

Naturally occurring surfaces are not fully planar. They often show some degree of roughness at the scale of optical wavelengths \cite{1,2,3,4,5}. This causes light incident upon them to be partly reflected away from the specular direction. The concept of gloss is related to the amount of light scattered into a small angular interval about the specular direction. When designing and manufacturing materials for which gloss is considered an essential parameter, it is desirable to know how this quantity is related to the surface topography, and in particular, to the parameters used to characterize them.

Gloss does in principle depend on any process that can scatter light away from the specular direction; e.g. surface and bulk randomness. In the present work, we will limit ourselves to situations where the bulk randomness can be ignored relative to the surface randomness. The gloss for randomly rough surfaces was recently studied experimentally \cite{6,7} and theoretically \cite{8} (see also Ref. \cite{9}). In this latter study, Alexander-Katz and Barrera derived, within the scalar Kirchhoff approximation, an expression for gloss for two types of surface height-height correlations (exponential and Gaussian). These authors stressed that it is important to \textit{not} neglect the incoherent contribution to gloss (stemming from the diffusely scattered light), since it may be significant. The publications \cite{8,9} are among the few studies found in the literature where also the surface correlation is included when trying to estimate gloss from the surface roughness parameters.

In this paper, we reexamine gloss of a randomly rough surface. An expression for this industrially relevant quantity is derived within the framework of phase-perturbation theory \cite{10,11}, for a general height correlation function. Like the authors of Ref. \cite{8}, it is found that the surface correlation is important for gloss in general. However, contrary to Alexander-Katz and Barrera \cite{8}, it turns out that in our formulation it is not the product of the correlation length and a lateral momentum variable (collection angle) that acts as one of the reduced variables for the estimation of gloss from surface parameters. Instead, one finds that the corresponding reduced variable depends on the \textit{functional form} of the correlation function satisfied by the parameter.
surface roughness, and not only its correlation length. Only in some limiting cases do we recover results consistent with Ref. [8].

When applying approximate expressions to calculate important optical quantities, it is of utmost importance to be able to have knowledge about the range of validity of the expression used. In order to address this crucial point, we use results from rigorous Monte Carlo simulations to gauge the quality of the proposed approximate analytical expression to gloss. To the best of our knowledge, such extensive comparison to rigorous simulation results has never been reported before. The main reason for considering a one-dimensional scattering geometry was to enable such a comparison. Rigorous simulation in this context of a two-dimensional geometry is out of reach for today’s computer power.

2 Gloss

In the optical industry, gloss is used extensively to quantify the visual appearance and functional properties of various materials [6, 8, 12, 13]. However, it does not show the same prominence in the optics branch of science where it is not-so-often considered. In fact, the term does not even have a rigorous scientific definition, and it comes in several “flavors”: specular and wide-angle gloss referring to different angles of incidence (20°, 60° and 85°) [13]. For instance, the way that gloss is quantified and measured (by gloss-meters) depends on industrial standards [13] that are different in, say, north-America and Europe. However, in essence, what the gloss numbers quantify, is how well a material scatter light incident upon it into the specular direction. Depending on the level of surface topography and/or inhomogeneities in the bulk of the material, a fraction of the incident light will be scattered into directions other than the specular. Such mechanisms will contribute to reduce the gloss numbers of such materials.

In this study, we will define gloss, $G(\theta_0)$, as the fraction of the incident light that is scattered into a small angular interval, $\Delta \theta$, about the specular direction.\footnote{Usually the normalization is \textit{not} done with respect to the total scattered energy, but instead relative to the (specular) reflectance of a smooth reference (black glass) material (that depends on the standard used). The authors of Ref. [8] adopted a normalization consisting of the reflectance of a smooth material of the same type as that being investigated. For not too rough surfaces, our definition follows closely the one by Alexander-Katz and Barrera since the total scattered energy is only moderately sensitive to the roughness.} This definition is not identical to any of the industrial standards in common use today [13]. However, it shares the main characteristics of these standards, and for appropriate choices of the angular interval can be related to them. Furthermore, we will be somewhat unorthodox and also consider “gloss” in transmission, even though it is not a commonly used term. The concept of haze is more customarily considered in this context [14].

3 The Scattering Geometry

The scattering geometry that we will consider in this study is depicted in Fig. 1 In the region $z > \zeta(x)$ it consists of vacuum ($\varepsilon_0(\omega) = 1$) and for $z < \zeta(x)$ of a dielectric medium characterized by an isotropic, frequency-dependent, dielectric function $\varepsilon_1(\omega)$. Here $\zeta(x)$ denotes the surface profile function, that is assumed to be a single-valued function of $x$ that is differential as many times as is necessary. Furthermore, it constitutes a zero mean, stationary, Gaussian random process that is defined by

$$\langle \zeta(x) \rangle = 0,$$

$$\langle \zeta(x)\zeta(x') \rangle = \sigma^2 W(|x - x'|).$$

Here $W(|x|)$ denotes the (normalized) auto-, or height-height correlation function, $\sigma$ is the root-mean-square of the surface roughness, and $\langle \cdot \rangle$ denotes the average over an ensemble of realizations of the surface roughness. For the discussion to follow one will also need the power spectrum of the surface roughness, defined as the Fourier transform of the correlation function, i.e.

$$g(|k|) = \int dx \ e^{-ikx} W(|x|).$$

\textcopyright 2003 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim
amount of roughness transfer of the scattering (or transmission) process into the specular direction. Hence, it does depend on the root-mean-square roughness associated with the surface topography and the perpendicular momentum.

It can be demonstrated that gloss of a randomly rough surface can be expressed as \[ G(\theta) = \frac{1}{U} \int_{\theta_-}^{\theta_+} d\theta \left\langle \frac{\partial U}{\partial \theta} \right\rangle, \] where \( \theta_\pm = \Theta \pm \Delta \theta \), with \( \Theta = \arcsin \left\{ \left( \sqrt{\varepsilon_m/\varepsilon_0} \right) \sin \theta_0 \right\} \) being the specular direction in reflection (\( \varepsilon_m = \varepsilon_0 \)) and transmission (\( \varepsilon_m = \varepsilon_1 \)). Moreover, \( U = \int_{-\pi/2}^{\pi/2} d\theta \left\langle \frac{\partial U}{\partial \theta} \right\rangle \) denotes the reflectance or transmittance of the rough surface. Within the framework of phase-perturbation theory \[10, 11, 14\], it can be demonstrated that gloss of a randomly rough surface can be expressed as \[ G(\theta) \approx \exp \left\{ -\sigma^2 \Lambda^2(k\langle k \rangle) \left( 1 - \frac{\alpha_0(q) \Delta q}{\pi} \right) \right\}, \] where \( k = \sqrt{\varepsilon_0(\omega/c)} \sin \theta_0 \) and \( \alpha_m(q) = \sqrt{\varepsilon_m\omega^2/c^2 - q^2} \) (\( \exists m \alpha_m > 0 \)). Moreover, in writing Eq. \[4a\], one has introduced a power spectrum dependent factor defined according to\[2\]

\[ G(a) = \frac{1}{2\Delta q} \int_{q_-}^{q_+} dq g(|q - k|) = \frac{1}{2\Delta q} \int_{-\Delta q}^{\Delta q} dq g(|q|), \] where \( q_\pm = k \pm \Delta q = \sqrt{\varepsilon_m(\omega/c)} \sin \theta_\pm \) with \( \Delta q = \sqrt{\varepsilon_m(\omega/c)} \cos \Theta \sin \Delta \theta \), and \( a \) denotes the correlation length.

There are several important observations that should be made from Eqs. \[4\]. First, gloss can be expressed in terms of two dimensionless quantities: \( \sigma \Lambda(k\langle k \rangle) \) and \( G(a) \Delta q \). The former is the product of the root-mean-square roughness associated with the surface topography and the perpendicular momentum transfer of the scattering (or transmission) process into the specular direction. Hence, it does depend on the “amount” of roughness but not on how it is being correlated along the interface. In quite a few studies of

\[2\] For an exponential and Gaussian correlation function characterized by the correlation length \( a \), one has \( G(a) = (2/\Delta q) \arctan(\Delta qa) \) and \( G(a) = (\pi/\Delta q) \text{erf}(\Delta qa/2) \), respectively, where \( \text{erf}(\cdot) \) denotes the error function.

Fig. 1 The scattering geometry used in this study. The rough surface is defined by \( z = \zeta(x) \). The region above the surface, \( z > \zeta(x) \), is assumed to be vacuum \( (\varepsilon_0(\omega) = 1) \), while the medium below is a dielectric characterized by a frequency-dependent dielectric function \( \varepsilon_\pm(\omega) \). Notice for which directions the angle of incident (\( \theta_0 \)), scattering (\( \theta_s \)), and transmission (\( \theta_t \)) are being defined as positive. An angle of transmission is only well-defined if the lower medium is transparent, i.e. if \( \Re \varepsilon_1(\omega) > 0 \).
gloss for rough surfaces, this is the only factor considered. The latter quantity, \( G(a)\Delta q \), on the other hand, depends on the form of the power spectrum and thus, indirectly, on the correlation length. Notice, however, that it is only the functional form of the power spectrum \( g(|q|) \) around zero (lateral) momentum transfer that enters into the expression for gloss via \( G(a) \). Second, the dependence of gloss on the angle of incidence only enters through the perpendicular momentum transfer present in \( \sigma\Delta k|k| \) (with \( k = \sqrt{\varepsilon_0(\omega/c)\sin \theta_0} \)).

For completeness, and to facilitate the use of these approximate expressions for gloss, we also give the full expressions in terms of the “defining” quantities. Gloss in reflection can be expressed as

\[
G_r(\theta_0) \approx \exp \left[ -16\pi^2\varepsilon_0 \left( \frac{\sigma}{\lambda} \right)^2 \cos^2 \theta_0 \left\{ 1 - 2\sqrt{\varepsilon_0} \frac{G(a)}{\lambda} \sin \Delta \theta \cos \theta_0 \right\} \right],
\]

while in transmission one has

\[
G_t(\theta_0) \approx \exp \left[ -4\pi^2\varepsilon_0 \left( \frac{\sigma}{\lambda} \right)^2 \left\{ \frac{\varepsilon_1}{\varepsilon_0} \sin^2 \theta_0 - \cos \theta_0 \right\}^2 \right.
\]

\[\times \left\{ 1 - 2\sqrt{\varepsilon_1} \frac{G(a)}{\lambda} \sin \Delta \theta \sqrt{1 - \frac{\varepsilon_0}{\varepsilon_1} \sin^2 \theta_0} \right\} \left\{ \sqrt{\varepsilon_0} - \sqrt{\varepsilon_1} \right\} \right],
\]

In obtaining the expression for \( G_t(\theta_0) \) it has been used that \( \cos \Theta_i = \sqrt{1 - (\varepsilon_0/\varepsilon_1) \sin^2 \theta_0} \) for the specular direction in transmission.

Previously, Alexander-Katz and Barrera \[8\], reported while using scalar Kirchhoff theory, that the reduced variables for gloss (in reflection) were \( (\sigma/\lambda) \cos \theta_0 \) and \( (a/\lambda)\Delta \theta \). Since in the radiative region \[4, 5\] \( \alpha_0(k) = \sqrt{\varepsilon_0(\omega/c)\cos \theta_0} \), it follows readily that \( \sigma\Delta k|k| \propto (\sigma/\lambda) \cos \theta_0 \). However, we do not in general find that \( G(a)\Delta q \) scales like \( a\Delta \theta \) (the product of the correlation length and the collection angle). Only in the limit \( a\Delta q \ll 1 \), for which \( G(a) \propto a \), do we recover the scaling reported by Alexander-Katz and Barrera \[3\]. Notice that for small collection angles one has \( a\Delta q \approx 2\pi \sqrt{\varepsilon_0} \cos \Theta (a/\lambda)\Delta \theta \). However, below we will see that when the ratio \( a/\lambda \) becomes rather small, the phase perturbative approximation to gloss becomes less accurate. Over the range of validity of this approximation we therefore find that for a one-dimensional roughness the reduced correlation dependent variable for gloss is \( G(a)\Delta q \) and not simply the product of the correlation length and the collection angle as reported in Ref. \[8\].

We will now address the accuracy of the analytic expressions for gloss derived in this work. This will be achieved by comparing these expressions to what can be obtained from rigorous Monte Carlo simulations \[4, 5\] that in principle takes all higher order scattering processes into account. The simulation results using an exponential correlation function (and assuming \( p \)-polarization for the incident light) are presented in Fig. \[2\]. They demonstrate that the approximate expressions are rather good even for relatively rough surfaces. Furthermore, they seem to produce the best results for \( a/\lambda \gtrsim 1 \) (and \( \sigma/\lambda \) not too large) for which one naively would expect single scattering to mainly contribute. Hence, for rough, shortly correlated surfaces where \( \sigma/a \gg 1 \) the approximate expressions presented herein are no longer adequate. Comparable, or better, results have been obtained for \( s \)-polarization. There is one important difference to be noticed between the results for \( p \) and \( s \)-polarization. In the former state of polarization, the Brewster angle phenomenon is present, and as a result causes the estimation of gloss to be rather sensitive \[3\] to angles of incidence about the Brewster angle (cf. Fig. \[2\](c)). However, for \( s \)-polarization, Eqs. \[4\] represent a good approximation to gloss over the entire range of angles of incidence.

5 Conclusions In conclusion, we have derived approximate analytic expressions to gloss within the framework of phase-perturbation theory. We found that the reduced variables for gloss are: (i) the root-mean-square roughness times the perpendicular momentum transfer for the specular direction, and (ii) a height-height correlation dependent factor times a lateral momentum transfer variable. These findings only

---

\[3\] The obtained results for gloss do also for such angles of incidence depend somewhat on the definition used for gloss.
Fig. 2 Gloss as a function of (a) the surface roughness $\sigma/\lambda$ for fixed $a/\lambda = 1.58$ and $\theta_0 = 0^\circ$; (b) the correlation length $a/\lambda$ for $\sigma/\lambda = 0.058$ and $\theta_0 = 0^\circ$; (c) the angle of incidence $\theta_0$ keeping $\sigma/\lambda = 0.058$ and $a/\lambda = 1.58$ fixed. The surface roughness used to obtain these results was a Gaussian random process characterized by an exponential correlation function, $W(x) = \exp(-|x|/a)$, of correlation length $a$. For all figures the wavelength of the $p$-polarized incident light was $\lambda = 0.6328 \, \mu m$ and $\Delta \theta = 2.5^\circ$. The open symbols are results of rigorous Monte Carlo simulations, while the solid lines are the predictions of Eqs. (4). The vertical dashed-dotted lines in Figs. 2(a) and (b) correspond to the assumptions made for $\sigma/\lambda$ and $a/\lambda$ in Figs. 2(b) and (a), respectively. Moreover, the vertical dash line in Fig. 2(c) corresponds to the position of the Brewster angle for the corresponding planar scattering geometry. Recall that in $s$-polarization the Brewster phenomenon is not present, and the prediction of Eqs. (4) is of good quality for the entire angle of incidence range.

References
[1] P. Beckmann and A. Spizzichino, The scattering from electromagnetic waves from rough surfaces, (Artech House, 1963).
[2] F.G. Bass and I.M. Fuks, Wave scattering from statistically rough surfaces, (Pergamon Press, Oxford, UK, 1979).
[3] J. A. Ogilvy, Theory of wave scattering from random rough surfaces (IOP Pub., Bristol, 1991).
[4] K.F. Warnick and W.C. Chew, Waves Random Media 11, R1-R30 (2001).
[5] I. Simonsen, A random walk through surface scattering phenomena: Theory and phenomenology, arXiv:cond-mat/0408017, 2004.
[6] R. R. Méndez, R. G. Barrera, and R. Alexander-Katz, Physica A 207, 137 (1994).
[7] L. Wang, T. Huang, M.R. Kamal, A.D. Rey, and J. Teh, Polymer Engineering & Science 40, 747 (2004).
[8] R. Alexander-Katz and R. G. Barrera, J. Polym. Sci. B: Polym. Phys. 36, 1321 (1998).
[9] J. O. Porteus, J. Opt. Soc. Am. 53, 1394 (1964).
[10] J. Shen and A. A. Maradudin, Phys. Rev. B 22, 4234 (1980).
[11] J. A. Sánchez-Gil, A. A. Maradudin, and E. R. Méndez, J. Opt. Soc. Am. A 12, 1547 (1995).
[12] M.E. Nadal and E.A. Thompson, Journal of Coatings Technology 72, 61 (2000).
[13] ASTM Standard D 523-89, Standard Test Method for Specular Gloss, 1989; ASTM Standard E 430-91, Standard Test Method for Measurement of Gloss of High-Gloss Surfaces by Goniophotometry, 1991.
[14] Ingve Simonsen et al. unpublished 2005.