

# Advanced Methods and Models for Describing Coating Appearance

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## Abstract

The National Institute of Standards and Technology has recently initiated a study to advance appearance metrology. A systems approach which applies technological advances in optical metrology, mathematical modeling, and computer rendering to the development of new methods of appearance characterization and to more accurate methods of modeling the appearance of coatings and coated objects will be used. Corresponding experimental and modeling research activities will be conducted in four areas: coating composition, microstructure of coating films, reflectance properties, and appearance descriptions. The parameterized mathematical models and computer rendering, when coupled with advanced measurements, will support the capability of researchers and engineers to assess the contribution of coating constituents to appearance and help design coatings with appropriate initial appearance and durability properties. This paper presents an overview of the planned research.

## Introduction

The appearance (color, gloss, texture) of a coated object greatly affects a customer's perception of the product's quality. Moreover, customer expectations for appearance attributes of coatings are continually increasing, as manufacturers demonstrate their ability to provide coatings having new and exciting appearance attributes [1]. The continued enhancement of appearance will require significant advances in metrology and predictive models.

Current appearance metrology is based primarily on specular and colorimetric measurements. This has led to a host of specialized metrics. Although these metrics are useful for some measurements, they are inadequate for describing coatings having reflectance properties that depend on the angles of illumination and viewing, for characterizing texture, for predicting the appearance of a finished product from the coating constituents, or predicting the appearance of a coating as the product ages.

Fortunately, recent advances in measurement and characterization procedures, modeling, computer rendering, and visualization are available and can be used to support improvements in appearance measurements and modeling. In response to recommendations by industry [2] and the Council of Optical Radiation Measurements [3], the National Institute of Standards and Technology (NIST) has initiated a project to advance appearance metrology. Four NIST laboratories are participating in this research. They are the Building and Fire Research, Information Technology, Manufacturing Engineering, and Physics Laboratories.

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## Overview of Appearance Project

In a systems approach, technological advances of the past three decades in optical metrology, mathematical modeling, and computer rendering will be applied to the development of new methods of quantitative appearance characterization and to more accurate methods of predicting the appearance of coatings and coated objects. The goals of this research are to:

- Develop advanced textural, spectral, and reflectance metrologies and models for quantifying the reflection of light from a coating film,
- Use the advanced metrologies to generate scattering maps and validate physical models describing optical properties of a coating, and
- Develop computer image rendering (creation) capability, based on either measurements or models, to systematically investigate relationships among optical properties and appearance and accurately predict the appearance properties of coated objects.

To meet these goals, research is planned in the four areas illustrated in Figure 1: i) coating composition, ii) microstructure of coating films, iii) reflectance properties, and iv) appearance description (e.g., scattering maps, appearance measurements, and computer rendering of an image). Each area has an experimental and a modeling component. Experimental results will be used to test model predictions and make refinements in models, as needed. Of key importance will be coordinating and linking results among the areas to reach the overall goal of predicting appearance from compositional data.

In the project's first year, the focus is on simple model coatings, namely clear rough coatings. Because the microstructure and reflectance properties are relatively simple in this case, it should be possible to both characterize and model the microstructure and reflectance properties of these coatings and to compare the experimental results with the model predictions. Pigmented coatings, including those having directional reflectance properties, will be investigated in future years.

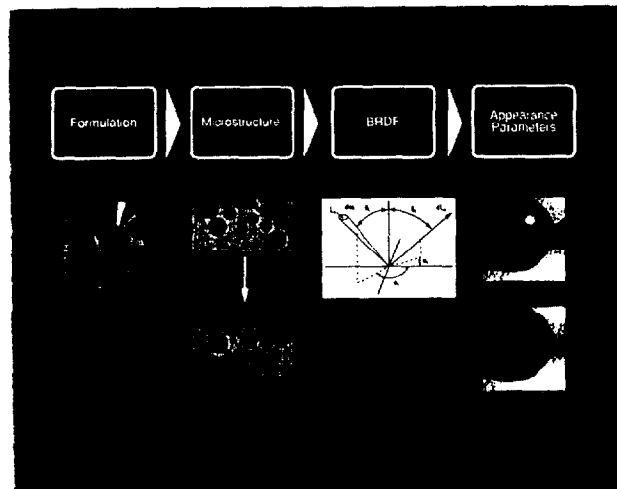


Figure 1. Schematic illustrating four research areas of the appearance study.

## Coating Composition

Coating composition together with application procedures, film formation processes and surface characteristics determine the appearance of a coating film [4,5]. To meet the project objectives, relationships between properties of the constituents of a coating and the microstructure and appearance of the film must be developed. Recently-developed technologies will be used to extend the manufacturer's characterization of the properties of coating constituents to meet these needs. Primary concerns include characterizing size, geometry, size distribution, volume concentration and dispersion of pigments in a coating. Field-flow fractionation, which has been used to characterize pigment and latex size distributions [6,7], is an example of a technique which will be investigated for use in this study.

## Microstructure of Coating Films - Experimental Characterization

The microstructure (the nature and distribution of phases) of new and aged coatings will be experimentally characterized using a combination of techniques. Experimental microstructure data are needed to test models for simulating microstructure from compositional data and to provide input for mathematical models for predicting optical properties of coatings.

Many techniques have been used to characterize the microstructure of coating films. For example, recent papers have discussed using atomic force microscopy (AFM) to characterize surface morphology of latex coatings [8,9]. Several techniques, including AFM, scanning acoustic microscopy and confocal laser microscopy, have been used to investigate defects in organic coatings [10]. Surface roughness has been characterized using mechanical profiling instruments [11-15] and optical techniques [11,16].

In this project, several techniques, including stylus profiling, white light interferometric microscopy, confocal microscopy and scanning electron microscopy will be used to characterize the microstructure of coating films. The stylus profiling technique provides data on surface morphology. It is expected that white light interferometric microscopy will also provide meaningful measurements of the topography as well as limited data on the subsurface structure, including the positions, sizes, and morphology of subsurface pigment particles. In this technique [17], a white light source is split into two beams near the objective. Part of the light passes through the objective to the sample, the other part passes through the objective to a mirror. Light beams reflected from the sample and the mirror travel back through the objective to a detector. A product signal is obtained and takes the form of an interference or fringe pattern. By analyzing the phase information in the fringes, depth measurements accurate to a fraction of a wavelength can be obtained [18].

Confocal scanning optical microscopy has also been used to characterize the topography of coatings [11]. It can also be used to obtain information on the positions, sizes, and morphology of subsurface pigment particles down to about 250 nm in diameter. A confocal microscope uses a laser to illuminate one point on the sample at a time. The reflected light passes back through the objective and through a pinhole. An image is built up point by point by scanning either the sample or the illuminating beam. When the point on the sample is out of focus, the reflected light is defocused and does not pass through the pinhole. In this way, reflected light is obtained from a narrow slice of the sample (z-slice) perpendicular to the light beam. By moving the sample stepwise in the z direction, a series of images is obtained which can be reconstructed to provide 3-dimensional data. Computer manipulation of the reconstructions can be used to provide many views of the sample.

In a preliminary study to investigate the use of confocal microscopy for characterizing the microstructure of coatings, images of a metallic base-coat/clear-coat automotive coating system and of a TiO<sub>2</sub>-pigmented alkyd coating were obtained. In Figure 2, two views of the metallic

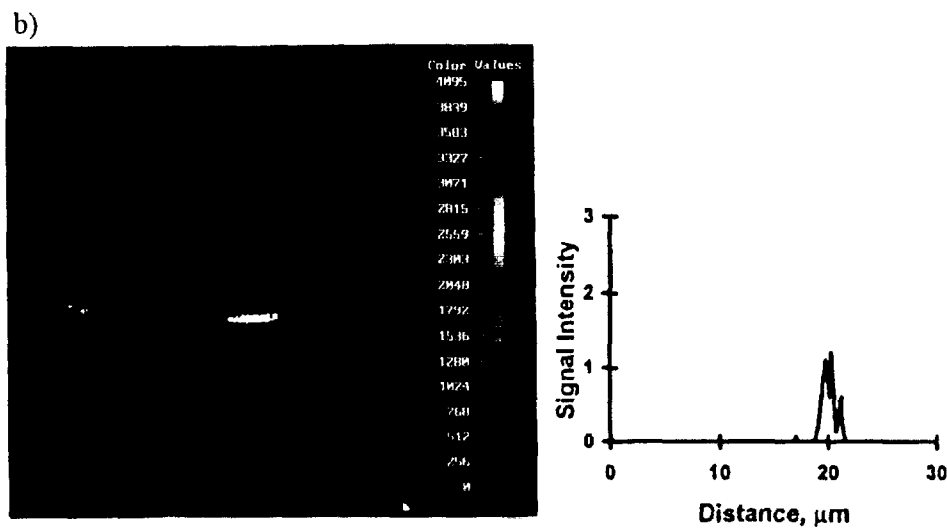
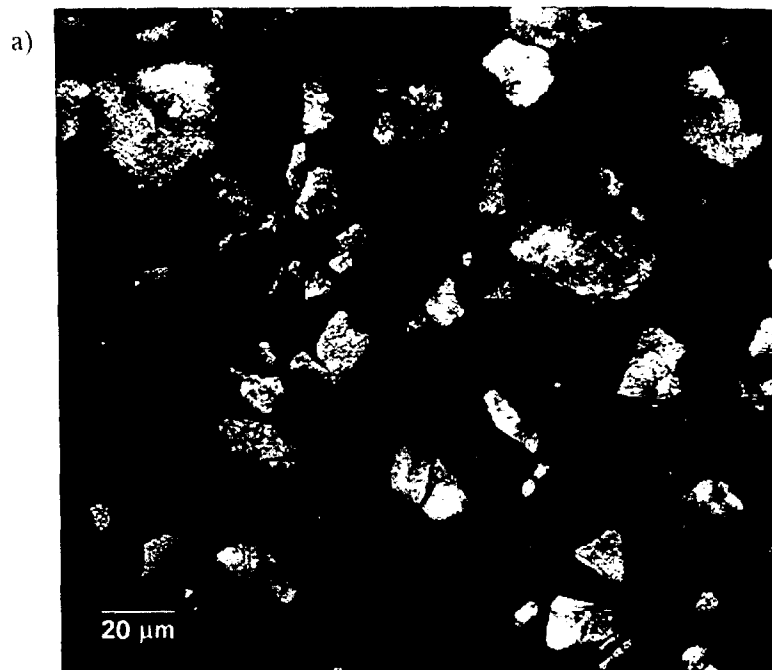


Figure 2. Confocal micrographs of an automotive metallic basecoat/clear-coat system. Figure 2a is an oblique view of a reconstruction of z-slice data showing the orientation and dispersion of the metallic flakes. Figure 2b is a cross-sectional view (x-z slice) of the same coating. Figure 2c is a plot of the integrated z-slice signal intensity as a function of distance from the surface of the coating for the x-z slice shown in 2b. The top of the coating (at the bottom of the photograph) is marked by highly reflective gold dust.

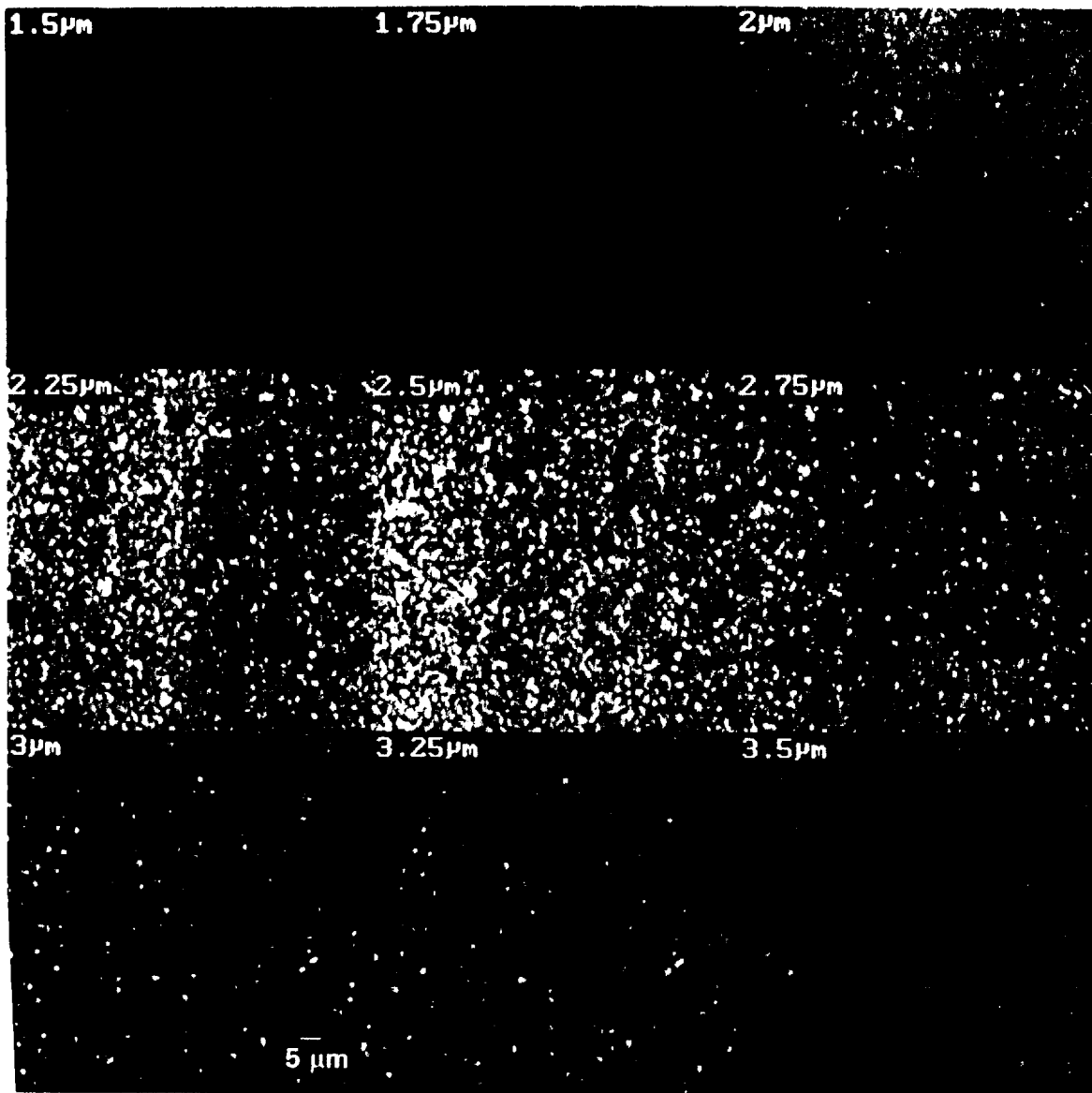


Figure 3. Confocal micrographs of z slices of a TiO<sub>2</sub> pigmented alkyd coating having a 4 percent pigment volume fraction. Relative positions of the z stage are noted in the upper left hand corner of the micrographs.

system are displayed. Figure 2a shows an oblique angular view of a three-dimensional reconstruction (maximum pixel intensity) of a set of reflected light images taken throughout the film thickness. Brighter areas in Figure 2a correspond with regions having higher reflectances. An optical cross section (x-z scan) of the same coating system is shown in Figure 2b. In this depiction, reflectance is obtained for a line within the field of view for slices perpendicular to the surface of the film. A small amount of fine gold dust was placed on the surface of the film (bottom of the illustration, indicated by an arrow) to aid the microscopist in locating the surface of the clear coat. A plot of intensity versus depth (z direction) for the image shown in Figure 2b is shown in Figure 2c. This plot indicates the thickness of the clear coat is about 19  $\mu\text{m}$ . Information from the base coat is obtained for a depth of about 3  $\mu\text{m}$ , although the total z-scanning distance was 25  $\mu\text{m}$ . Depths greater than about 22  $\mu\text{m}$  appear to be hidden by the overlying pigments.

Figure 3 shows 250 nm thick z-slices of a  $\text{TiO}_2$ -pigmented oil-based coating. The pigment volume concentration of the film is 4 percent. The numbers in the upper-left hand corner indicate a relative position of the z stage. Because gold dust or other material was not used to mark the film surface, it is not clear that the first image is of the coating surface. Pigments are just visible in the second image and throughout the remaining images. Based on these micrographs, it appears that limited 3-dimensional information can be obtained to describe pigment distribution in a coating film.

In addition to evaluating the microstructure of coating films using these three techniques, cross sections will be characterized using electron microscopy. Mathematical procedures [e.g., see 19] will also be used to model 3-dimensional microstructure data based on 2-dimensional experimental data and the results compared with confocal microscopic data.

### Microstructure - Modeling

Microstructural models of coating films are needed to provide the link between compositional data and reflectance modeling. As with the other areas, existing work can be applied. For example, relationships between the nature of surface defects in pigmented organic coatings and gloss have been analyzed [20]. Surface-defects formation [5], leveling of thixotropic coatings [21], and polymer phase separation [22] during film formation have been investigated. As for placing pigments within a film, a mathematical model has been developed to predict the effects of extenders on pigment dispersion in coating films [23]. Particle packing in pigmented latex films has been modeled [24]. Hunt, Martin and Galler [25] at NIST have simulated microstructure of coating films in conjunction with a study on photo-degradation of coatings.

The two-dimensional simulation modeling was carried out to investigate the relationships between coating composition parameters and gloss loss upon aging [25]. For this model, it was necessary to develop a parametric procedure to distribute pigments within the film. The parameters included in the model are pigment size, pigment shape (spherical or disk shaped), pigment volume (area) content, and pigment dispersion.

In the present model, pigment particles are distributed in one of two ways: randomly placed or placed according to a Poisson point process which simulates clustering or flocculation. Figure 4a shows a cross-section of an unaged film having random placement of pigments of five sizes with a 2-dimensional volume (area) content of 25 percent. Figure 4b shows the film after simulated photo-degradation. Figures 5a and 5b illustrate corresponding unaged and aged films in which the pigment is flocculated. Although limited data were analyzed, features of the simulations and actual cross sections of coating films appear similar (23, 26).

Data describing the microstructure, obtained both from experimental characterization of coating films and from simulation models, will be used in reflectance models. It is evident that the ability to describe the microstructure of a film parametrically is an essential link between coating composition and appearance rendering.

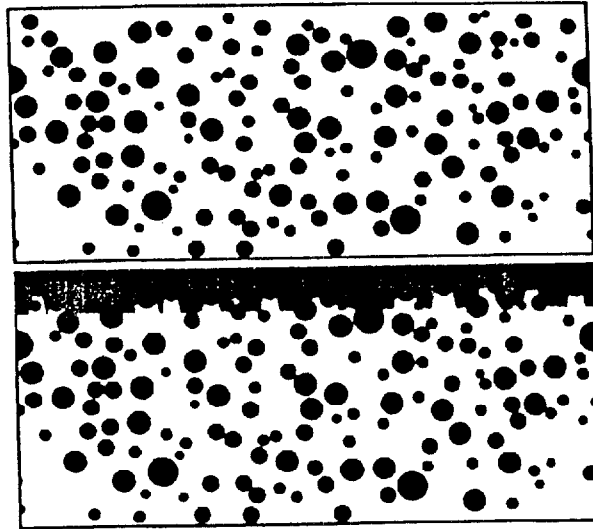


Figure 4. Two-dimensional simulation of photodegradation of a coating having a pigment volume concentration of 25 percent with no pigment flocculation. Figure 4a represents a section perpendicular to the surface of an unaged coating while Figure 4b shows the section after it has been photo-degraded.

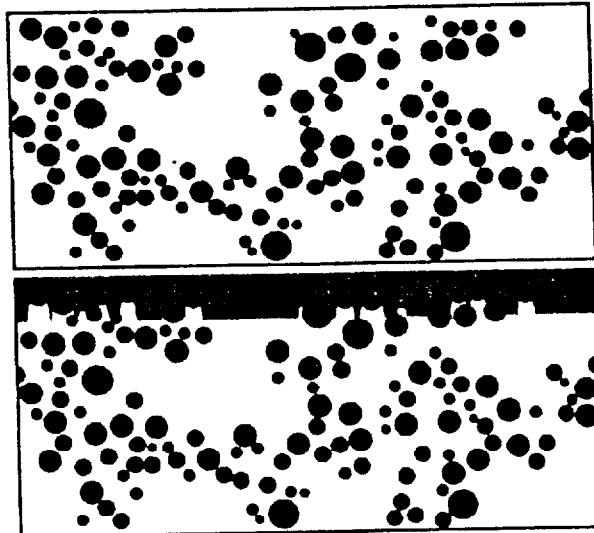


Figure 5. Two-dimensional simulation of photodegradation of a coating having a pigment volume concentration of 25 percent with pigment flocculation. Figure 5a represents a section perpendicular to the surface an unaged coating while Figure 5b shows the section after it has been photo-degraded.

## Reflectance Properties of Coated Objects - Experimental Characterization

Characterizing the reflectance properties of a coated object is complex. This is because reflectance depends on the angle of the incident light on the surface, the spectral distribution of the incident light, the observing angle, the area under observation, and the physical properties of the sample.

The mathematical function which captures this information is called the bidirectional reflectance distribution function (BRDF) [27]. Assuming that the scattering properties of the sample are uniform and isotropic, the BRDF,  $f_r$ , can be written as

$$f_r(\theta_i, \phi_i, \theta_r, \phi_r, \lambda_i) = dL_r(\theta_i, \phi_i, \theta_r, \phi_r, \lambda_i) / [L_i(\theta_i, \phi_i, \lambda_i) \cdot \cos \theta_i \cdot d\omega_i]$$

where  $L$  is radiance, the subscript "i" refers to the incident beam, the subscript "r" refers to reflected beam,  $E_i$  is the incident irradiance,  $\lambda$  is wavelength, and the angles are defined as shown in Figure 6.

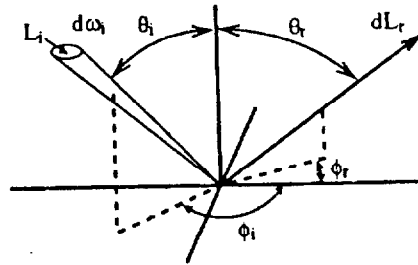


Figure 6. Schematic illustration of the bi-directional reflectance distribution function (BRDF).

Traditionally, except for in-plane goniophotometers and instruments designed to measure haze (reflectance a few degrees about the specular angle [28]) and orange peel, the use of directional reflectance information has been limited. Hammond [29] noted, for example, that it was only practical to measure specular reflectance for one direction of illumination. More recently, it was stated that specular reflectance is often determined for only one or two angles of illumination [30]. To help overcome these practical limitations, reflectance is often treated as consisting of two distinct phenomena – regular or specular reflection and diffuse reflection. This has led to a host of specialized metrics [31] that apportion the two phenomena to obtain an acceptable measurement sensitivity for a particular appearance need. However, in practice, it is often not possible to separate the two phenomena because the reflectance is too complex.

Directional reflectance curves are continuous. They range from the delta-function spikes of highly specular surfaces to the smooth flat curves of Lambertian surfaces [32] and also include a wide variety of distorted shapes that do not fall directly between the two extremes. Thus, to meet the needs of characterizing materials whose reflectance properties depend upon the angles of illumination and viewing, or improving characterization of texture and haze, more complete characterization procedures are needed.



Recent advances have been made in measurement techniques to more completely characterize reflectance. This is illustrated by McCamy's recent review of instruments for measuring directional coating appearance properties [33] and a new spectral tri-function automated reference reflectometer (STARR) built at NIST [34]. STARR is capable of measuring spectral reflectance at incidence angles up to 80° from sample normal over a wavelength range of 200 nm to 2500 nm. It is used in preparing standard reference materials, carrying out calibration measurements, and meeting other reflectance measurement needs. The instrument is computer controlled and can be programmed to obtain reflectance data over the range of angles and wavelengths with only minimal need for operator involvement.

For this project, it is planned to measure reflectance using existing NIST instruments and to construct a new reflectance measurement instrument. It is planned to have goniometric, spectral and imaging capabilities to accommodate material specific geometries. Additionally, because coatings may fluoresce as well as reflect light, an instrument to measure fluorescence is also being considered. All of the instruments will be of sufficient sensitivity and accuracy to develop measurement transfer standards.

### **Reflectance Properties of Coated Objects - Modeling**

The measured reflectance properties will be used as input for comparisons with other measures of appearance, for computer rendering of images, and for validating reflectance models. The proposed numerical approach to derive BRDF from the measured coating topography and microstructure is based on electromagnetic theory. A statistical model for the light scattered from the coating will be derived from a series of elementary calculations of the light scattered from a single particle in a dielectric binder using integral equations equivalent to Maxwell's equations. The statistical model will take into account the roughness of the dielectric surface, and the size distribution and location of the particles. Computer codes have been developed to calculate rigorously the scattered field from a rough perfect conductor [35], a rough dielectric interface [36], and two neighboring dielectric spheres [37]. Additional codes will be developed for a sphere in a rough dielectric layer and a sphere in a rough interface. An approximate model of the interaction of the light with the surface and the distribution of particles in the coating will be developed by summing the scattered light intensities from each interaction. The validity of this approximation will be evaluated by performing a rigorous calculation for light scattered from a small number of particles and then comparing this result with that obtained by adding the intensities of the scattering from each of the particles.

Once an accurate model for scattering from coatings is developed, the results will be used as input BRDFs for surface image renderings and numerical estimates of appearance parameters from measurements of the surface topography and coating microstructure.

### **Scattering Maps and Appearance Measurements**

The objective of the experimental part of research in this area is to develop comparisons between detailed BRDF data and other appearance measuring devices instruments. The details will be developed as BRDF instruments are developed and data become available.

### **Computer Rendering**

Over the past 15 years, there has been great interest in computer graphics in generating realistic synthetic images, that is rendering. In particular, extensive efforts have been made to develop algorithms for rendering physically-accurate images—that is, images computed from numerical descriptions of a scene that accurately show what the scene would look like if it were built. Examples of rendered images abound on the internet and in the computer graphics literature. As

an example, Dorsey and Hanrahan [38] present rendered images to illustrate the development of patina on a small statue of a Buddha.

There are three interrelated classes of data that are important to computer rendering: geometry, radiometry, and materials. Although images can be, and often are, rendered using simple models for reflectance and illumination, more accurate descriptions are needed to predict true appearance [39].

In principle, the spectral BRDF for each of the objects in a scene would provide the basis for physically-accurate computer image rendering. The effects of some important parameters could be investigated including lighting conditions and direction of viewing. However, because of the number of parameters that must be selected (e.g., angular resolution) in obtaining BRDF data, many questions remain about specific procedures to use in characterizing the BRDF of a coated surface and in representing the data for rendering programs. Rendering studies could provide a means of systematically investigating some of these issues. For example, surfaces could be rendered using complete and censored BRDF data and the appearance of the objects compared.

### Summary

The National Institute of Standards and Technology has recently initiated a study to advance appearance metrology. The proposed research is a systems approach to appearance metrology, which will apply technological advances in coating characterization, optical metrology, mathematical modeling, and computer rendering to the development of new methods of quantitative appearance characterization and to more accurate methods of modeling the appearance of coatings and coated objects from coating constituents. Improvements in appearance metrology are important because of needs for more quantitative measurements of optical properties of coated objects, for development of new coatings, and for adequately describing optical properties of coatings having reflectance properties that depend on the angles of illumination and viewing. Parameterized mathematical models will be developed to describe coating films and predict reflectance properties. Model predictions will be verified with appropriate experimental measurements. The measurements and models data will be used in computer rendering programs to investigate relationships among coating parameters, reflectance properties and appearance.

### Acknowledgments

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