# Correlation of Predicted and Observed Optical Properties of Multilayer Thermal Control Coatings

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## Abstract

Thermal control coatings on spacecraft will be increasingly important, as spacecraft grow smaller and more compact. New thermal control coatings will be needed to meet the demanding requirements of next generation spacecraft. Computer programs are now available to design optical coatings and one such program was used to design several thermal control coatings consisting of alternating layers of $WO_3$ and $SiO_2$. The coatings were subsequently manufactured with electron beam evaporation and characterized with both optical and thermal techniques. Optical data were collected in both the visible region of the spectrum and the infrared. Predictions of solar absorptance and infrared emittance were successfully correlated to the observed thermal control properties. Functional performance of the coatings was verified in a bench top thermal vacuum chamber.

# Introduction

Thermal control in spacecraft will be increasingly important, as spacecraft grow smaller and more compact. Such spacecraft with low thermal mass will have to be designed to retain or reject heat more efficiently. Although there are many thermal control coatings available in today's market, new thermal control coatings will be needed to meet the demanding requirements of next generation spacecraft. Computer programs, now available for the modeling of thin film optical properties, can be used to predict thermal control properties.

The optical properties of interest for predicting thermal control performance are spectral absorptance and spectral emittance. Absorptance over the range of the solar spectrum can be used to calculate solar absorptance, a measure of the fraction of the incident sunlight that is absorbed. Spectral emittance over the range of a given blackbody spectrum can be used to calculate infrared emittance, a measure of how much a thermal control coating rejects heat to space relative to a perfect emitter. To calculate both solar absorptance and infrared emittance, it is necessary to have optical properties data from the ultraviolet to the infrared, nominally from 250 nm to 14 microns.

The objectives of this work are to utilize a currently available computer program to design several multilayer thermal control coatings, to deposit the multilayer coating systems of interest using electron beam evaporation, to characterize the final products for their thermal control properties, and to compare the observed results with the predictions obtained from the software. Achieving these objectives will lead to utilizing the predictive capabilities of modeling to identify the prospective performance of new thermal control coating systems.

## Methods

No single thermal control coating is ideal. Thermal control coatings are tailored to a particular application. In most cases, thermal control coatings are used to cool an object in space. This is achieved by a design that rejects heat efficiently to the surroundings and absorbs little heat from the surroundings. One example of such an application is the body of the Hubble Space Telescope. Other examples include the radiators for space power systems. To accomplish this task, a high emittance dielectric coating transparent in the visible region of the spectrum is placed on top of a low absorptance (high reflectance) layer. The low absorbing (high reflecting) layer is a metal, such as aluminum or silver, often deposited on a smooth polymeric substrate.

Silver was selected here as the reflective coating for the model. The transparent coatings selected for the model were $WO_3$ and $SiO_2$, deposited individually or in alternating layers over the reflecting silver layer. All three coatings can be deposited using electron beam evaporation or some other physical vapor deposition technique. Considered infinitely thick by the model, the silver was deposited to an actual thickness of about 100 nm on polished quartz substrates. Thicknesses for $WO_3$ and $SiO_2$ were varied during modeling, and specific thicknesses were identified for electron beam evaporation.

The optical properties of $SiO_2$ are particularly suited for low absorptance, high emittance applications owing to the transparent nature of the material in the visible and the absorbing nature of the material in the infrared. The optical properties of $WO_3$ are also suited for low absorptance, high emittance applications, being nearly transparent in the visible and somewhat absorbing in the infrared. Tungsten oxide is also of interest owing to its potential use in electrochromic applications [1].

Because the $WO_3$ and $SiO_2$ coatings were to be deposited on top of a silver reflective layer, it was necessary to identify the desired deposition thickness of each. Electron beam evaporated coatings tend to spall if they exceed 500 nm. Hence, a practical upper limit for oxide coating thickness was set at 400 nm, on 100 nm of silver. The coatings were deposited in an Eratron Model EB-8 electron beam evaporator. A Leybold Inficon, Inc. Model XTC quartz crystal monitor was used to monitor film thickness during deposition, and a Sloan Dektak II profilometer was used to quantify film thickness on witness coupons after deposition.

## Optical Properties Modeling

The program selected for optical properties modeling was TFCalc™, a product of Software Spectra, Inc., Portland, OR. Values for the refractive index, n, and extinction coefficient, k, as a function of wavelength, were needed for each material as input to the modeling program. Values for $SiO_2$ were obtained from Palik [2], while values for crystalline $WO_3$ were obtained from Hale [3]. The n and k values for both materials extend from 250 nm to 14 microns.

The criteria used to select optimal coating thickness from the modeling program was low absorptance in the visible and high absorptance in the infrared, as viewed in a plot of absorptance versus wavelength.

Spectral absorptance values are necessary but not sufficient to calculate solar absorptance, $\alpha_s$. The calculation requires that the spectral absorptance values be weighted by intensity values from the air mass zero (AM0) solar spectrum. Hence, low spectral absorptance in the visible yields a low $\alpha_s$.

Spectral absorptance values are necessary but not sufficient to calculate infrared emittance, $\varepsilon$. Kirchhoff's law dictates that absorptance equals emittance, at each wavelength

[4]. The spectral absorptance (i.e. spectral emittance) values from the TFCalc™ program were used in a spreadsheet to calculate total emittance for each sample. The calculation was performed according to Siegel and Howell [4], where total emittance is calculated based on the spectral emittance of the desired coating combination weighted by the spectral intensity of a given blackbody. In this case, the given blackbody spectrum was from a blackbody at 300 K. The absorptance data were averaged over 1 micron increments for the calculation.

Figure 1 shows the AM0 solar spectrum and the 300 K blackbody spectrum used to normalize the spectral absorptance data.

The presence of the silver layer below the $WO_3$ and $SiO_2$ dielectric coatings allowed a direct comparison of the predicted spectral reflectance of the selected coatings and the actual spectral reflectance, as measured by a spectrophotometer and infrared reflectometer.

## Optical and Thermal Performance Evaluation

Optical performance evaluation of the coatings was carried out using a Perkin Elmer Lambda-9 spectrophotometer equipped with a 15 cm diameter integrating sphere [5] and a Gier-Dunkle DB-100 infrared reflectometer [6], at room temperature. Total reflectivity data were collected in the range of 250 to 2500 nm with the spectrophotometer, representing much of the solar spectrum. Reflectivity in the vicinity of 9 microns was obtained with the DB-100. A functional evaluation of thermal performance was obtained from a bench top thermal vacuum chamber. This chamber is used routinely to make low temperature calorimetric vacuum emittance (LCVE) measurements in the range of 150 to 350 K [7].

## Results

Based on the criteria set above (i.e. low absorptance in the visible and high absorptance in the infrared) and the thickness limit set above (i.e. 400 nm for the dielectric coatings), the following multilayer coatings were selected for deposition and evaluation:

(a) 100 nm of $SiO_2$ and 300 nm $WO_3$,

(b) 300 nm of $WO_3$ and 100 nm of $SiO_2$, and

(c) 50 nm $WO_3$, 50 nm $SiO_2$, 100 nm $WO_3$, 50 nm $SiO_2$, and 150 nm $WO_3$,

each on 100 nm Ag.

The thickness of the $SiO_2$ layers measured by a profilometer matched the quartz crystal monitor thickness values. However, the thickness of the $WO_3$ layers exceeded the quartz crystal monitor thickness values by several percent. The as-deposited thickness values for the three selected samples were as follows:

(a) 100 nm of $SiO_2$ and 350 nm $WO_3$,

(b) 366 nm of $WO_3$ and 100 nm of $SiO_2$, and

(c) 64 nm $WO_3$, 50 nm $SiO_2$, 120 nm $WO_3$, 50 nm $SiO_2$, and 180 nm $WO_3$,

each on 100 nm Ag. Calculations from the TFCalc™ program were updated with the actual thickness values to facilitate comparison with observed optical properties.

TFCalc™ has as its output the optical properties of absorptance, reflectance, and transmittance. Reflectance was selected to provide a visual comparison between results predicted by the model and results actually measured on samples prepared by electron beam evaporation. Figure 2 compares the predicted and observed results between 250 and 2500 nm. Fair agreement was obtained on samples (a) and (c).

Figure 3 shows the spectral absorptance data obtained from the model, for the three candidate multilayer coating combinations, out to 14 microns.

Table I summarizes the calculated solar absorptance of the three candidate substrates. Tabulated along with the calculated solar absorptance is the actual solar absorptance observed by the lambda-9 spectrophotometer. All values represent solar absorptance at AM0.

Table II summarizes the calculated infrared emittance. Tabulated along with the calculated emittance is the actual emittance observed by the DB-100 infrared reflectometer and the low temperature calorimetric vacuum emissometer.

## Discussion

Uncertainty in the observed solar absorptance from the spectrophotometer measurements is estimated to be ± 0.005. Although the predicted solar absorptance values fall outside of this range, they are considered in fair agreement with the observed solar absorptance values. The calculated values do not match the observed values exactly, however, they are probably adequate for the purpose of estimating thermal control coating performance. One way to improve the correlation between calculated and observed values is to use in the modeling program n and k values that represent exactly the electron beam evaporated $SiO_2$ and $WO_3$ used to manufacture the coatings. Ellipsometry is considered an excellent technique for obtaining sample specific n and k values.

Uncertainties in the observed infrared emittance values from the DB-100 and LCVE measurements are estimated to be ± 0.005 and ± 0.010, respectively. Although the calculated infrared emittance values fall outside of this range in some cases, they are also considered in fair agreement with the observed infrared emittance values. Again, the calculated values are probably suitable for use in estimating thermal control coating performance.

For a 300 K blackbody, measurements out to 14 microns encompass 51.6% of the blackbody curve. To improve the correlation between calculated and observed values, it will be important to utilize n and k values out to 25 microns (83.4% of the blackbody curve), or more. In this way, a greater portion of calculated spectral emittance values would be available for normalizing the 300 K blackbody curve. Sample specific n and k values may also provide a more exacting correlation between calculated and observed emittance values. It is interesting to note that there is good agreement between the DB-100 and LCVE measurements.

## Conclusions

Optical modeling of several $WO_3$ and $SiO_2$ multilayer coatings was accomplished using a commercially available modeling program. Absorptance values obtained from the program were used to calculate the optical properties of solar absorptance and infrared emittance by convoluting the absorptance data into the air mass zero solar spectrum and the 300 K blackbody spectrum, respectively. Electron beam evaporation was used to manufacture the $WO_3$ and $SiO_2$ multilayer coatings to the same specifications as those used in modeling. A comparison of calculated solar absorptance and infrared emittance values with observed solar absorptance and infrared emittance values gave fair results, adequate for predicting the thermal performance of candidate thermal control coatings. Improvements to the modeling should improve the correlation between calculated and observed solar absorptance and infrared emittance.

## Acknowledgements

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Table I Solar absorptance, predicted and observed.

|  | Solar Absorptance |  |
|---|---|---|
| Sample | Predicted | Observed |
| A | 0.177 | 0.198 |
| B | 0.191 | 0.155 |
| C | 0.196 | 0.228 |

Table II Infrared emittance, predicted and observed, at 300 K.

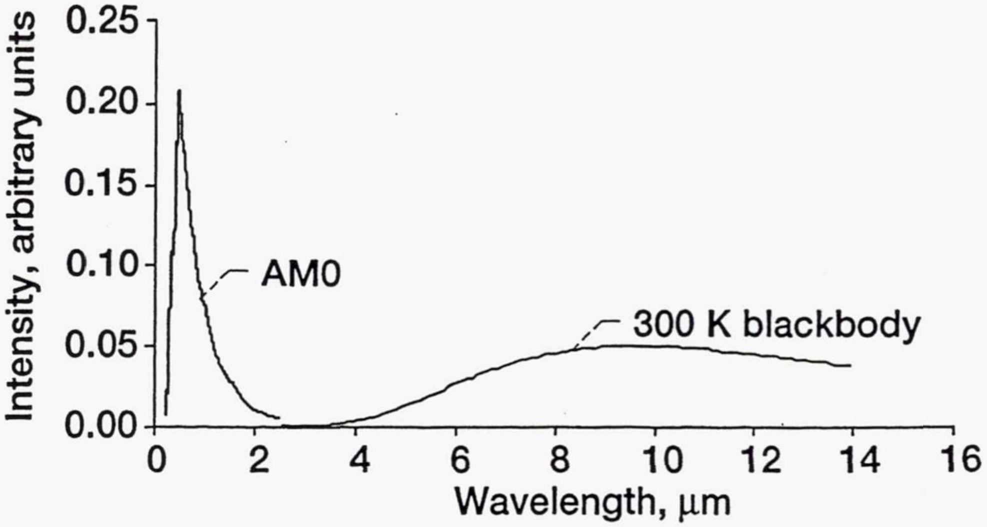
| | Infrared Emittance | | |
|---|---|---|---|
| Sample | Predicted | DB-100 | LCVE |
| A | 0.074 | 0.059 | 0.069 |
| B | 0.083 | 0.093 | 0.100 |
| C | 0.082 | 0.048 | 0.080 |

# Figure Captions

Figure 1 Spectral intensity of the air mass zero solar spectrum and 300 K blackbody spectrum, from 0.250 to 14 microns.

Figure 2. Calculated reflectance compared to the observed reflectance for: (a) 100 nm Ag/100 nm $SiO_2$/350 nm $WO_3$, 100 nm Ag/366 nm $WO_3$/100 nm $SiO_2$, and (c) 100 nm Ag/64 nm $WO_3$/50 nm $SiO_2$/120 nm $WO_3$/50 nm $SiO_2$/180 nm $WO_3$.

Figure 3. Calculated absorptance for: (a) 100 nm Ag/100 nm $SiO_2$/350 nm $WO_3$, (b) 100 nm Ag/366 nm $WO_3$/100 nm $SiO_2$, and (c) 100 nm Ag/64 nm $WO_3$/50 nm $SiO_2$/120 nm $WO_3$/50 nm $SiO_2$/180 nm $WO_3$.



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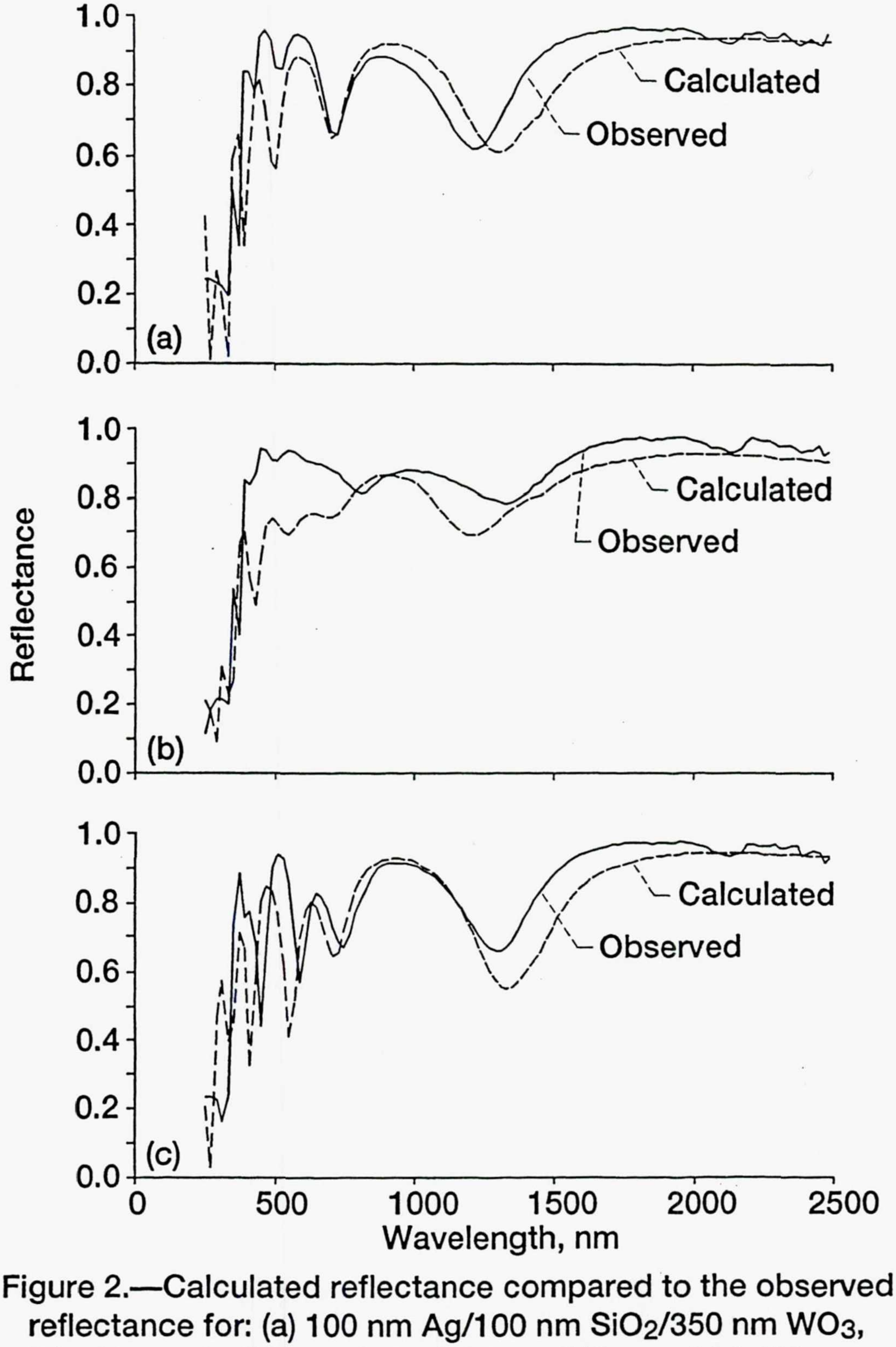

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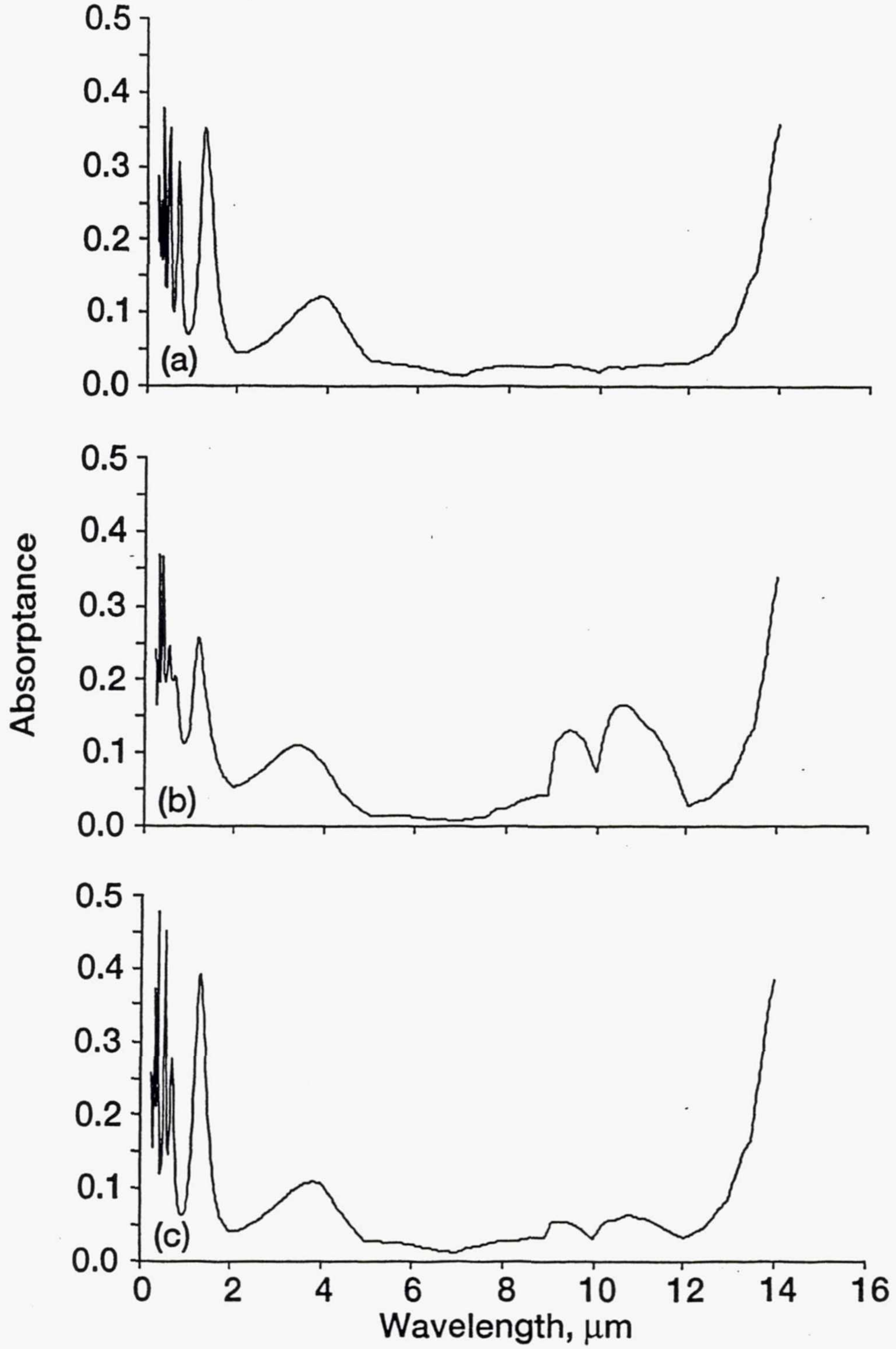

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