COMPUTATION OF TOTAL HEMISPHERICAL EMISSIVITY FROM DIRECTIONAL SPECTRAL MODELS

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Abstract:

Kirchoff's law and experimentally obtained data and/or theory (such as from Drude's model) for optical constants have been used in a modified geometric optics approximation (GOA) to obtain directional spectral emissivity. Then this spectral emissivity is used to obtain the total hemispherical emissivity by integration over direction and spectral range as weighted by the Planck distribution. The computations account for surface dependencies on temperature, composition, and roughness. The computed results for both the spectral directional and the total hemispherical emissivity are compared with the available data for platinum, stainless steel 304, and tungsten surfaces.

Keywords: Total hemispherical emissivity, Monte Carlo, Emittance, Geometric Optics Approximation

1 Introduction

Spectral directional emissivity, which describes emissivity at particular wavelengths and directions, depends on a variety of factors in addition to wavelength and direction. These additional factors would include material composition, surface oxidation, surface roughness, and surface temperature, among others. Total hemispherical emissivity is an integral of the spectral emissivity over all directions and all wavelengths. For accurate evaluation of heat transfer at very high temperatures, it would be ideal if total hemispherical emissivity could be obtained from a first-principles based approach (most likely grounded in Electromagnetic Theory and Maxwell's Equations) where all of the dependencies mentioned above are accounted for. This would extend predictive capability far beyond that of the limited sources of existing experimental literature. Some conventions use emittance as the emissivity of non-ideal surfaces, but for simplicity, emissivity is used as a catch-all term throughout this work.

Total hemispherical emissivity can be obtained from experimental data or from experimentally observed trends and relations [1][2]. In some cases, theory is indeed applied to culminate into a total hemispherical emissivity such as has been done by Rosenberg et. al[3], however, this is limited to the case of idealized, flat, unoxidized surfaces. Despite the importance of total hemispherical emissivity in high temperature systems, theoretical models describing the effects of roughness, oxidation, etc., have yet to be developed.

Greater progress in the application of theory however has been made regarding spectral and spectral directional emissivity. First, the acquisition of experimental data is relatively easier than in the case of total hemispherical emissivity. Spectral directional emissivity is measurable directly by means of infrared spectroscopy while total hemispherical emissivity can rely on either integrating a large amount of spectral direction data or through a delicate calorimetric setup. Furthermore, through Kirchhoff's Law, spectral directional emissivity can be obtained through spectral directional reflectance. For spectral directional reflectance, the sample does not require the same sort of environmental isolation or signal considerations needed for direct emission measurement. Not only does Kirchhoff's Law make experimental work easier, it also means that a large body of theoretical work dedicated to spectral directional reflectance is immediately transferrable to spectral directional emissivity. While challenges remain, many techniques and methods have been developed and are still being refined in modeling spectral directional emissivity. Various approaches are being taken to resolve effects such as temperature dependence, roughness and surface oxidation.

The effect of temperature on total emissivity is two-fold. The Planck Distribution, which describes the distribution of wavelengths comprising total emitted light (of a blackbody), is temperature dependent. Shifts in temperature will shift the Planck Distribution, thereby changing the ratio of emissive power given off by any given finite wavelength range to the total emitted power. This is the most immediate influence that temperature has on total emissivity, but the temperature can also influence the optical and dielectric constants of the material thus influencing the spectral directional emissivity. Several theoretical models have been developed to describe the optical constants within certain ranges of wavelength, material, and temperature, for example, the Hagen-Rubens Relation[4], Drude Model[5], Lorentz Model, Lorentz-Drude Model[6], Brendel-Bormann Model[7], Drude-Roberts[8] and the dampened Drude model developed by Chen and Ge[9]. Models such as Lorentz and Brendel-Bormann are generally better suited to dielectric materials whereas the Drude Models and the Hagen-Rubens Relationship (which follows the Drude Model) are more suited to metals. Additional measures beyond the Drude model must be taken in order to describe the anomalous skin region[10] or the interband absorption in noble metals[11]. Critical reviews of different models of optical constant for different application spaces and ranges of validity although the most general of expression of optical constants are available in open literature [12][13]

For a roughened surface, Wen and Mudawar [14] demonstrated how simple roughness factors developed by Agababov[15][16][17] could be implemented to achieve good experimental agreement for spectral emissivity of aluminum surfaces. Theoretically in-depth methods have also been developed focusing on the interaction of light with the surface. These methods would include using electromagnetic theory and Maxwell's equations or ray-tracing methods to evaluate some input surface profile. Unfortunately, the field of surface metrology is still open and there is not yet a generally-agreed upon method of characterizing and mathematically representing a real surface. However, modeling efforts have found reasonable success by utilizing pseudorandomly-generated Gaussian-distributed surface profiles [18][19]. Generally, a rigorous method of generating spectral directional emissivity for a non-ideal (roughened, patterned, etc.) input surface would be the direct solving of Maxwell's equations through means such as the Finite-Difference Time-Domain method, Finite Elements, or Rigorous Coupled Wave Analysis. There exist several prewritten scripts and software programs that implement one of these approaches to solving

Maxwell's Equations, for example, MEEP[20] and Georgia Tech's RCWA[21], have been used for this very purpose. However, direct solving methods require significant computational resources compared to simpler methods such as ray-tracing. This is especially true for pseudorandom surface profiles as opposed to repeating structures (structures such as grating geometries or smooth cavities) if meshing is to be considered for a method such as Finite Elements.

For a rough surface, the region of physical validity of the Geometric Optics Approximation (GOA, also referred to as Geometric Optics, Geometric Optics Ray-tracing, Ray-tracing, and GO) has been studied by various authors. The GOA approach saves computational resources by tracing the interaction of ray of light with surface instead of solving Electromagnetic and Maxwell's equations. Tang and Dimenna identified several parameters having strong influence on the accuracy of the GOA method, namely incident angle, ratio of root mean square (rms) deviation to correlation length and the ratio of the rms deviation to wavelength[22] and produced a regime map based on the latter two parameters. Fu and Hsu identified additional dependency of incident angle and produced an updated regime of validity including all three parameters[23]. Both of these studies focused on one-dimensional roughness. As computational capabilities have increased, so has the ability to model more complex geometries, such as two-dimensional surfaces. Both Tang[24] and Bergström et al [25] investigated the ray tracing of 2D Gaussian random rough surfaces and found minor differences compared to a similar models of 1D geometry. While the GOA method is limited at high incident angles, recent work has shown the capability of the RCWA method to match experimental data in such conditions.[26]

The addition of a thin dielectric layer (such as an oxide layer) can add further complication by introducing interference effects. Several authors have found reasonably effective ways of dealing with this as well. Iuchi modeled emissivity of oxidized metal by treating the oxide layer and the metal substrate as parallel, ideal, layers[27]. This method was capable of including interference effects which can be particularly distinctive in the example of iron oxidation[28]. The method of Phase ray-tracing attempts to include interference effects within the framework of the GOA method. This method was used by Lee et al. [29] to model gold and silicon oxide coatings on a silicon substrate. Further evaluation of the method identified limitations and the necessity to normalize associated calculations due to the violation of energy conservation[30]. More recently, a similar method, dubbed Hybrid Partial Coherence and Geometric Optics (or HPCGO), was developed by Qiu and Wu and compared to Maxwell equation solving methods[31]. Zhang and Zhao[32] included interference effects in their GOA adaptation, although the interference effects included in their model address multiple reflections on the surface of a single layer rather than the interference effects associated with multiple layers.

As discussed, there are a variety of physics-based techniques that can be used in the attempt to resolve several dependencies in the formulation of a spectral directional emissivity. In general, the models previously discussed produce discrete spectral directional emissivity (or reflectance) values or they produce a bi-directional reflectance distribution function (BRDF) which can then in turn be integrated to give discrete values of spectral directional emissivity.

This study presents the simple concept of generating a total hemispherical emissivity coefficient by iteratively running a spectral directional emissivity model for directions and wavelengths representative of what would be expected in nature. The spectral directional emissivity model accounts for dependencies of wavelength, direction, composition, temperature and roughness and so the total hemispherical emissivity captures the desired dependencies of composition, temperature and roughness as well. While the spectral directional model presented in this paper is not theoretically fundamental, it still demonstrates that the accounting of dependencies at the spectral directional level can propagate through to a total hemispherical emissivity.

Of the many modeling techniques reviewed, the GOA was chosen for several reasons. First, it is a flexible, straightforward technique that can be internally authored and altered. This way, it could easily be written to be looped for Monte Carlo sampling purposes, which is proposed in this research as a methodology of generating a total hemispherical emissivity coefficient from a spectral directional emissivity model. Secondly, it is not particularly computationally intensive and so the sampling method could be explored with quicker turnaround time. Thirdly, Monte Carlo ray-tracing methods are already commonly used to model radiative heat transfer in complex systems that may not be solvable deterministically. It was expected that the established method of sampling energy bundles[33] could be applied analogously to spectral directional models, such as the GOA, to derive a total hemispherical emissivity.

Nomenclature

Abbreviations

GOA	Geometric Optics Approximation
RCWA	Rigorous Coupled Wave Analysis
FDTD	Finite Difference Time Domain
MEEP	MIT Electromagnetic Equation Propagation
BRDF	Bi-directional Reflectance Distribution Function

Expressions

L, l	Surface profile length
λ	wavelength
T	temperature
k_b	Boltzmann constant
B	blackbody spectral radiance
σ	Stefan-Boltzmann Constant
k	imaginary refraction index
R	reflectivity
r	reflection ratio
n	real refractive index
Ω	solid angle
θ	zenith angle
ϕ	azimuthal angle
A	Area
σ_R	RMS roughness factor
p	probability
S	Period shift
Ψ	Model roughness parameter
ε	Emissivity or Emittance

Subscripts

$\perp$	s-polarization (perpendicular)
$\parallel$	p-polarization (parallel)
i	incident
N	normal incidence
λ	spectral

2 Theory

Emissivity is a thermodynamic property of a material (surface), but its first principle computation is difficult. Here, we use a model that utilizes Kirchhoff's law relating spectral and directional emissivity to reflectance, and optical constants of the material. In short, the model progresses as follows: A wavelength is selected by sampling the Planck Distribution. Then, many light rays at this wavelength are simulated against an input surface at various angles of incidence and at various different locations along the surface profile. Spectral directional emissivity can be related to spectral directional reflectance through Kirchhoff's Law and so this produces a set of spectral directional emissivities. This set can then be integrated to obtain total spectral emissivity of the surface at this wavelength. A new wavelength is sampled and the procedure is repeated to obtain total spectral emissivity at the new wavelength. Once the Planck Distribution has been sampled sufficiently, the total spectral emissivity values may be averaged to yield a total hemispherical emissivity.

The evaluation method of total spectral emissivity used in the GOA follows figure 1. This model differs slightly from several other GOA adaptations in that BRDF's are not used and spectral directional values are pursued directly.

Figure 1. The progression of the GOA towards a spectral emissivity. The first step (1) involves projecting a ray of light onto the input surface and evaluating for the reflected and absorbed intensity. The Fresnel equations at the particular spot on the profile are used for this evaluation, as explained in section 2.1. The second step (2) involves starting the incident ray at a new location on the plane of incidence and performing the same progression. The average of satisfactorily many evaluated starting locations, uniformly distributed across the incident plane, yields the directional emissivity for that surface as explained in section 2.2. A new incident angle is evaluated in the third step (3). At this new incident angle, a new spectral directional emissivity is evaluated using steps (1) and (2). An adequate number of directional emissivity may be integrated to yield a total spectral emissivity as explained in section 2.3. [Please format to 1 column width]

2.1 Evaluation of $\epsilon(s, \lambda, \theta, T)$ at a surface point s

At an individual surface point s , spectral directional emissivity is obtained in accordance with Kirchhoff's Law

$$\epsilon(s, \lambda, \theta, T) = 1 - R(s, \lambda, \theta, T) \quad (1)$$

It is also assumed that Kirchhoff's Law is valid for the two different polarizations of light.

$$\epsilon(s, \lambda, \theta, T) = \frac{1}{2}(\epsilon_{\perp} + \epsilon_{\parallel}) \quad (2)$$

$$\epsilon_{\parallel} = 1 - R_{\parallel} \quad (3)$$

$$\varepsilon_{\perp} = 1 - R_{\perp} \quad (4)$$

The reflection coefficients for each polarization are found by

$$R_{\perp 2} = R_{\perp 1} * r_{\perp} \quad (5)$$

$$R_{\parallel 2} = R_{\parallel 1} * r_{\parallel} \quad (6)$$

Where $R_{\perp 1}$ and $R_{\parallel 1}$ represent the relative intensities of the incident s-polarized and p-polarized light, respectively. Meanwhile, $R_{\perp 2}$ and $R_{\parallel 2}$ represent the corresponding relative intensities of the reflected s-polarized and p-polarized light. The new ray could in theory reflect again on the surface somewhere. If this occurs, new values of $R_{\perp 2}$ and $R_{\parallel 2}$ are simply calculated using the most recently calculated $R_{\perp 2}$ and $R_{\parallel 2}$ input as $R_{\perp 1}$ and $R_{\parallel 1}$ into equations 5 and 6. The very first $R_{\perp 1}$ and $R_{\parallel 1}$ (original incident values) are set to 1. The $R_{\perp 2}$ and $R_{\parallel 2}$ coefficients found for the final ray to strike the surface are input into equation 4 for $R_{\perp}$ and $R_{\parallel}$.

Terms r_s and r_p may be calculated according to Eq.'s 7 and 8, found in page 98 of Howell [12]

$$r_{\perp} = \frac{a^2 + b^2 - 2a \cos(\theta) + \cos^2(\theta)}{a^2 + b^2 + 2a \cos(\theta) + \cos^2(\theta)} \quad (7)$$

$$r_{\parallel} = r_{\perp} \frac{a^2 + b^2 - 2a \sin(\theta) \tan(\theta) + \sin^2(\theta) \tan^2(\theta)}{a^2 + b^2 + 2a \sin(\theta) \tan(\theta) + \sin^2(\theta) \tan^2(\theta)} \quad (8)$$

Where coefficients a and b are

$$a^2 = \frac{1}{2} \left\{ \left[(n_{\lambda}^2 - k_{\lambda}^2 - \sin^2 \theta)^2 + 4n_{\lambda}^2 k_{\lambda}^2 \right]^{\frac{1}{2}} + n_{\lambda}^2 - k_{\lambda}^2 - \sin^2 \theta \right\}$$

$$b^2 = \frac{1}{2} \left\{ \left[(n_{\lambda}^2 - k_{\lambda}^2 - \sin^2 \theta)^2 + 4n_{\lambda}^2 k_{\lambda}^2 \right]^{\frac{1}{2}} - (n_{\lambda}^2 - k_{\lambda}^2 - \sin^2 \theta) \right\}$$

Temperature and wavelength dependencies of $\varepsilon(\lambda, \theta, T)$ are related to the temperature and wavelength dependencies of n and k. However, oftentimes the temperature dependency of the optical constants may be neglected. The angular dependency of $\varepsilon(\lambda, \theta, T)$ originates from equations 7 and 8.

2.2 Evaluation of $\varepsilon(\lambda, \theta, T)$ across the surface

The spectral directional emissivity, $\varepsilon(\lambda, \theta, T)$, of the surface is determined by the emissivity of each point on the surface and so

$$\varepsilon(\lambda, \theta, T) = \frac{1}{A} \int^{Surface} \varepsilon(s, \lambda, \theta, T) dA \quad (9a)$$

In the model, equation 9a is approximated by 9b over a 1D surface (single-variable function).

$$\varepsilon(\lambda, \theta, T) = \frac{1}{l} \int_0^l [1 + f'(x)^2]^{\frac{1}{2}} \varepsilon(x, \lambda, \theta, T) dx \approx \frac{1}{N} \sum_i^N \varepsilon(s_i, \lambda, \theta, T) \quad (9b)$$

Where $f(x)$ defines the 1-D surface over $x \in (0, l_p)$ and l is the real area (length of the surface). N is assumed to be sufficiently large for a good average over the surface. We have chosen $N > 100$. For smooth model input surfaces, N does not need to be very large to achieve good convergence, but for rougher input surfaces, a larger N may be required.

2.3 Evaluation of $\varepsilon(\lambda, T)$

Integrating $\varepsilon(\lambda, \theta, \phi, T)$ over all solid angle gives $\varepsilon(\lambda, T)$ according to equation 10.

$$\varepsilon(\lambda, T) = \frac{1}{\pi} \int \varepsilon(\lambda, \theta, \phi, T) \cos \theta d\Omega \quad (10)$$

If $\varepsilon(\lambda, \theta, \varphi, T)$ is equivalent across the azimuthal angle φ , (10) can be simplified to:

$$\varepsilon(\lambda, T) = 2 \int_0^{\frac{\pi}{2}} \varepsilon(\lambda, \theta, T) \sin \theta \cos \theta d\theta \quad (11a)$$

We have used the rectangular rule for integration:

$$\varepsilon(\lambda_j, T) \approx \frac{2}{N} \sum_{k=0}^N \varepsilon(\lambda_j, \theta_k, T) \sin(\theta_k) \cos(\theta_k) \quad (11b)$$

Where

$$\theta_k = \frac{\pi}{2} * \frac{k}{N+1}$$

And N is taken as 89 to for uniform sampling at one degree intervals. One could of course use any other quadrature rule or the Monte Carl method for integration.

2.4 Evaluation of $\varepsilon(T)$

The total hemispherical emissivity is obtained from a further integration over the Planck distribution via 12a.

$$\varepsilon(T) = \frac{\int_{\lambda=0}^{\infty} \varepsilon(\lambda, T) B(\lambda, T) d\lambda}{\sigma T^4} \quad (12a)$$

For most dielectrics and metals, the dominant effect that temperature has on $\varepsilon(T)$ manifests from the inherent temperature dependence of the Planck Distribution. For the remainder of this paper, shifts in temperature that shift the Planck Distribution will be referred to as Planck shifts. So the total hemispherical emissivity is given as

$$\varepsilon(T) \approx \lim_{M \rightarrow \infty} \frac{\sum_{j=1}^M \varepsilon(\lambda_j, T)}{M} \quad (12b)$$

Where the λ 's are generated through Monte Carlo sampling of the Planck Distribution. M is taken as sufficiently large (100 or so). The error bars represent the standard deviation amongst these calculated total values.

3 Model Results

The modeling of compositional, temperature, and roughness dependencies is approached sequentially. The final model, which attempts to demonstrate how each dependency can be accounted for in a total hemispherical emissivity coefficient calculation, includes a few deliberate steps of adjustment and extension. However, the model is built progressively to enable validation for each step individually. Each case is used to calculate normal spectral emissivities followed by spectral directional emissivities and then finally total hemispherical emissivities. In each case, comparisons are made with available experimental data where possible and total hemispherical emissivities always account for Planck shifts. Conveniently, the GOA method can still be applied to a flat surface and so comparison and validation can be achieved prior to the modeling of rough surfaces. For flat surfaces, it is relatively easy to produce an analytical or numerical solution of the surface since any given point along the flat surface is representative of the surface as a whole.

The model is started as GOA of a flat platinum surface so that it could be compared to existing and reliable literature. Platinum is a relatively chemical inert material and so unintended effects of chemical reactions that may have occurred in experimental studies ought to be limited. In this case, dependency on composition, and consequently, dependency on associated optical constants. Here, the optical constants are taken from the Rakic [11] where optical constants were generated by fitting the data acquired by Weaver[34] using the Lorentz-Drude model. Temperature dependence of the optical constants is neglected since

Silvera has suggested that the optical constants of platinum within the infrared wavelength range remain relatively constant across temperature.[35]

The second case of the GOA introduces Drude theory for stainless steel and tungsten in the attempt to capture temperature dependency in optical constants in addition to composition dependency and Planck shifts. Here, the optical constants are not assumed constant across temperature. The results are compared to the work of Rosenberg et al. [3] whose analytical model also uses Drude theory to derive temperature-dependent model inputs in the same manner for a flat surface.

The third case of the GOA attempts to mimic effects of roughness in addition to composition dependency. It is well established that the GOA method loses validity for directional spectral values at higher incident angles. It is shown in the spectral directional output during the first and second cases that p-polarized light is greatly overestimated as incidence approaches 90 degrees. A $\tan(\theta)$ term is introduced to roughly represent the high angle scattering effects that are typically neglected with the GOA method. The pseudo-random Fourier series surface profile is used and, once again, platinum is used as a benchmark and secondary temperature dependencies of the optical constants are neglected. The same references used in the first case are used again for optical constant input.

The final case of the GOA combines the optical temperature dependency accommodations of the second case with the roughness dependency accommodations of the third case. Drude theory is once again used to derive the optical constants and pseudorandom Fourier series profiles are used to characterize the surface. The $\tan(\theta)$ term is used to account for high angle scattering. Surfaces of stainless steel 304 and tungsten are modeled. The four cases are summarized in Table 1.

Table 1. Details of Presented Model Evaluations for each of the four Cases [Please format to 1.5 column width]

Case	Surface Composition	n, k Derivation Method	Emissivities Evaluated	Dependencies and Effects Accounted for during Evaluation
1	Pt	Experiment	$\epsilon_N(\lambda)$	Composition, λ , Polarization
			$\epsilon_{\parallel}(\theta, \lambda)/\epsilon_N(\lambda), \epsilon_{\perp}(\theta, \lambda)/\epsilon_N(\lambda)$	Composition, λ , Polarization, θ
			$\epsilon(T)$	Composition, λ , Polarization, θ , $B_{\lambda}(\lambda, T)$
2	ss304, W	Drude Theory	$\epsilon_{\parallel}(\theta, \lambda, T)/\epsilon_N(\lambda, T), \epsilon_{\perp}(\theta, \lambda, T)/\epsilon_N(\lambda, T)$	Composition, λ , Polarization, θ , T
			$\epsilon(T)$	Composition, λ , Polarization, θ , T, $B_{\lambda}(\lambda, T)$
3	Pt	Experiment	$\epsilon_N(\lambda)$	Composition, λ , Polarization, Roughness
			$\epsilon_{\parallel}(\theta, \lambda)/\epsilon_N(\lambda), \epsilon_{\perp}(\theta, \lambda)/\epsilon_N(\lambda)$	Composition, λ , Polarization, θ , Roughness
			$\epsilon(T)$	Composition, λ , Polarization, θ , $B_{\lambda}(\lambda, T)$, Roughness
4	ss304, W	Drude Theory	$\epsilon_{\parallel}(\theta, \lambda, T)/\epsilon_N(\lambda, T), \epsilon_{\perp}(\theta, \lambda, T)/\epsilon_N(\lambda, T)$	Composition, λ , Polarization, θ , T, Roughness
			$\epsilon(\theta, T)$	Composition, λ , Polarization, θ , T, $B_{\lambda}(\lambda, T)$, Roughness
			$\epsilon(T)$	Composition, λ , Polarization, θ , T, $B_{\lambda}(\lambda, T)$, Roughness

3.1 Case 1: Flat Platinum Surface

Optical constants are taken from Rakic's fitting of the data compiled by Weaver[34]. These experimental measurements were taken at temperatures either unreported, or significantly below that of Rolling and Silvera (250 °C in the case of the work of Seignac[36]). It is important to acknowledge the potential for variation in experimental measurements of platinum emissivity and other materials. Variations in experimental literature may be attributed to varying measurement methodologies, varying specimen surface roughness, and actual sample purity. Using a consistent polishing procedure as well as a consistent measurement methodology, Jain demonstrated that the total emissivity of platinum gathered from different sources, each claiming 99.9% purity or better, could vary by as much as 20%.[37] This variation in Jain's study was hypothesized to have originated from erroneous purity classification by suppliers. Experimental studies on the optical constants of a material are subject to the same potential sources of error found in emission studies using radiometric methods.

First, normal spectral emissivity coefficients are calculated and compared to experimental literature (Fig. 2). Model output aligns well with the experimental work of Silvera[35] and Aksyutov[38]. Consistency between the data points of Silvera, Aksyutov and the model supports the notion of temperature-independent optical constants of platinum. Slight variation is found in Rolling's[39] work at shorter wavelengths, however, rougher samples in the work of Rolling tended to have greater values at lower wavelengths.

Fig. 2. Results of modeling of normal spectral emissivity coefficients of platinum. The model assumes temperature independence. Good agreement is achieved between the model and the experimental works of Silvera and Rolling. Model values tend to be slightly less than experimental values. [Please format to 1 column width]

Relative spectral directional emissivity coefficients are evaluated and compared to the experimental work of Rolling. Figure 3 shows the evaluation of the parallel-polarized component of light across angle for several wavelengths while Figure 4 shows the same for the perpendicular-polarized component of light. The parallel component shows large increases at longer wavelengths and has maximum peak between 80 and 90° while the perpendicular component remains unchanged across wavelengths and decreases as the angle increases. Both of these trends are visible in the experimental literature as well as in the model output. However, the model tends to slightly overestimate the intensity of emitted parallel-polarized light. As mentioned previously, the GOA method does not perfectly resolve scattering at high angles of incidence.

Fig. 3. Parallel Component of Platinum Relative Directional Spectral Emissivity Coefficients through various wavelengths. Rolling experimental (left) and model output (right) both show increases at longer wavelengths, particularly at higher angles of incidence. [Please format to 2 column width]

Fig. 4. Perpendicular Component of Platinum Relative Directional Spectral Emissivity Coefficients. Rolling experimental (left) and model output (right) both show little to no change across wavelength. [Please format to 2 column width]

The model is Monte Carlo – sampled according to the Planck Distribution to generate total hemispherical emissivity coefficients across temperature. This comparison is given in Fig. 5. Although variation can occur between experimental results, the current model well predicts the tendency of experimental results.

Figure 5. Model and Experimental values [40][41][42][43][37][39] for total hemispherical emissivity of platinum. [Please format to 1.5 column width]

3.2 Case 2: Flat 304 SS Surface

The model is used once again for a flat, uniform surface profile and compared to experimentally derived relative spectral directional emissivity coefficients for both polarizations. Rather than use literature values of optical constants, the optical constants are now derived using Drude theory as is done by Rosenberg et al. [3]. The benefit to Drude is that it accounts for temperature dependence of the optical constants. The presented model is compared to Rosenberg's work to demonstrate convergence to a closed-form method in the case of a flat surface.

The relative spectral directional emissivity coefficients are once again evaluated and compared to the experimental work of Rolling[39]. Figure 6 shows the evaluation of the parallel polarized component of light across angle for several wavelengths while Figure 7 shows the same for the perpendicular polarized component of light. Both of the tendencies observed in the experiments are visible in the model output. However, the model tends to still overestimate the intensity of emitted parallel-polarized light at high angles of incidence as well as predict a greater angle of peak parallel emissivity.

Figure 6. Parallel Component of 304 Stainless Steel Relative Directional Spectral Emissivity Coefficients. Rolling experimental, $\sigma = .33\mu\text{m}$ (left) and model output (right) both show increases at longer wavelengths, particularly at higher angles of incidence. $T = 953\text{ }^\circ\text{K}$. [Please format to 2 column width]

Figure 7. Perpendicular Component of 304 Stainless Steel Relative Directional Spectral Emissivity Coefficients. Rolling experimental $\sigma = .33\mu\text{m}$ (left) and model output (right) both show little to no change across wavelength. $T = 953\text{ }^\circ\text{K}$. [Please format to 2 column width]

Model output is compared to the work of Rosenberg (Figure 8). Excellent agreement is achieved between the two methods implying practical convergence in the ideal scenario of a flat, homogenous surface.

Figure 8. Total hemispherical emissivity coefficients of SS 304 and Tungsten. Values are generated through Monte Carlo-sampled GOA for a smooth surface and are compared to the output of Rosenberg. [Please format to 1 column width]

3.3 Model setup for roughened surfaces

The model output resembles previous experimental results and converges to closed-form methods in the case of smooth surfaces. From here, two additional aspects are pursued: 1) The effect of surface roughness and 2) The limits of the model at high incident angles.

3.3.1 Pseudorandom surface profile generation

The surface profile consists of the sum of 30 cosine waves generated randomly according to equation 13:

$$f(x) = \sum_{i=1}^{30} \alpha_i \cos(\beta_i x + S_i) \quad (13)$$

Where

$$\alpha_i = \alpha^* r_{i,1}$$

$$\beta_i = \beta^* r_{i,2}$$

$$S_i = S^* r_{i,3}$$

Where all r_{ij} are pseudorandomly sampled values from a uniform distribution between 0 and 1, and

α^* is defined by β^* and Eqn. 14

$$\beta^* = \frac{500\pi}{L}$$

$$S^* = 2\pi$$

Traditionally, the surface generation typically used in directional spectral emissivity modeling techniques involves pseudorandom Gaussian profiles. However, the emphasis of this work is to demonstrate the sampling methodology rather than develop a perfect directional model. For this reason, the Fourier series approach was taken for the sake of convenience in code development. Adherence to a Gaussian height distribution is not checked. Each parameter is generated from pseudorandom sampling of a user-defined range of values having a uniform probability distribution. Each parameter set (e.g. amplitudes) has the same sampling range. The roughness of the profile is therefore dictated by the ratio of the amplitude sampling range to the period sampling range. The significance of this designation is that the model output is dependent on the relative geometric characteristics of the surface profile geometry rather than the actual dimensions of the surface profile. It has been suggested that the slope of the surface profile, rather than the profile amplitude, is the more-significant contributing parameter for emissivity [44] [45]. Furthermore, work in 3-D GOA modeling has emphasized the importance of rms slope above surface profile height/amplitude [25]. By altering the amplitude-to-period ratio via the ratio of the parameter sampling ranges, the model falls in accordance with this trend. To this end, β^* is held fixed at an arbitrarily large value to ensure adequate variation in the sample profile and α^* is the independent variable of the simulation.

Therefore, the value that characterizes the “roughness” of the generated profile is given as

$$\Psi = \alpha^* \beta^* \quad (14)$$

For more intuitive profile generation, it may be desirable in the future to uniformly sample the profile period ($1/\beta^*$) rather than the inverse period (β^*). During total hemispherical emissivity calculations, a new profile having the same defined Ψ is generated for each new λ .

3.3.2 High-angle scattering

The GOA method was found to consistently overestimate the relative spectral directional emissivity at high angles in the first two cases. For this reason, a small correction was included to try and account for the expected inaccuracies of the GOA method at higher incidence angles.

Originally, the model used the following equation:

$$\varepsilon(\lambda, \theta, T) = 1 - R(\lambda, \theta, T) \quad (15a)$$

Where $R(\lambda, \theta, T)$ is calculated through the GOA model. To account for additional scattering at higher angles, R evaluated by the GOA is replaced.

$$\varepsilon(\lambda, \theta, T) = 1 - R^*(\lambda, \theta, T) \quad (15b)$$

Where

$$R^*(\lambda, \theta, T) = \zeta + (1 - \zeta)R(\lambda, \theta, T)$$

Where

$$\zeta = \gamma \tan(\theta) (1 - H[\theta - \theta^*]) + H[\theta - \theta^*]$$

And

$$\theta^* = \tan^{-1}\left(\frac{1}{\gamma}\right)$$

$$\gamma = .01 - .02$$

This correction only significantly impacts coefficients at high angles of incidence, and does so while keeping the reflection coefficient between 0 and 1. This correction is used for the third and fourth cases.

3.4 Case 3: Roughened Platinum Surface

It is well established that the GOA approach is limited at high angles of incidence and for certain roughness-to-wavelength ratios. The two additions of the model (inclusion of the ζ high angle term and the introduction of a Fourier-series model profile) give additional quantitative resemblance to spectral directional emissivity values. As shown in Table 2, at very low Ψ (roughness) values, the normal spectral emissivity values approach the previous model case of the smooth surface as shown in Table 2. As Ψ increases, normal spectral emissivity values slowly increase, as would be expected from nature.

Table 2. Normal Spectral Emissivity Coefficients. [Please format to 1 column width]

λ [μm]	Flat Profile (It. 1)	$\Psi = \frac{\pi}{200}$	$\Psi = \frac{\pi}{40}$	$\Psi = \frac{\pi}{10}$
1.5	0.235424	0.235424	0.235432	0.241282537
3	0.100355	0.100355	0.100358	0.103065057
6	0.03455	0.03455	0.034551	0.036974646

The model is compared to available literature for relative spectral directional emissivity values in both parallel and perpendicular components of light at various roughness scales for two wavelengths (1.5 and 6 μm). As seen in figures 9a and 9c as well as 10a and 10c, the observed trends in the literature are consistent for both wavelengths; the relative parallel component experiences a decrease from increasing roughness, observed near peak angles while the perpendicular component experiences an increase from increasing roughness, observed at approximately the same angle range. The model outputs in figures 9b and 9d as well as 10b and 10d resemble this trend in roughness where three different Ψ values are used.

Figure 9. Parallel Component of Emitted Light from (a) Rolling at $\lambda = 1.5 \mu\text{m}$ and (b) model output at $\lambda = 1.5 \mu\text{m}$ and from (c) Rolling at $\lambda = 6 \mu\text{m}$ and (d) model output at $\lambda = 6 \mu\text{m}$. Several roughness scales were evaluated. [Please format to 2 column width]

Figure 10. Perpendicular Component of Emitted Light from (a) Rolling at $\lambda = 1.5 \mu\text{m}$ and (b) model output at $\lambda = 1.5 \mu\text{m}$ and from (c) Rolling at $\lambda = 6 \mu\text{m}$ and (d) model output and at $\lambda = 6 \mu\text{m}$. Several roughness scales were evaluated. [Please format to 2 column width]

Just as in previous cases, hemispherical emissivity coefficients across temperature and the comparison are shown in Figure 11. According to equations (11a) and (11b), the high- and low- incidence angle directional emissivity coefficients have relatively less contribution to the overall emission due to the sin and cos terms. There is relatively little change between the model values in Figures 5 and 11.

Figure 11. Model and Experimental values [40][41][42][43][37][39] for total hemispherical emissivity of platinum. Model inputs of $\Psi = \pi/40$ and $\gamma = .02$ were used. [Please format to 1 column width]

3.5 Case 4: Roughened SS 304 Surface

In the fourth case, the Fourier-series profile is used with the ζ correction factor while Drude Theory is used to derive the optical constants. This time, there is much better agreement between the model and literature in regards to the parallel-polarized component of relative emitted light from polished stainless steel 304 compared to case 2. The results are provided in Figure 12. The perpendicular component remained unchanged between the two cases, indistinguishable from Figure 7.

Figure 12. Parallel Component of Relative Spectral Directional Emissivity of polished stainless steel 304 at 953 °K and $\sigma = 0.33\mu\text{m}$. (left) and model output where $T = 953^\circ\text{K}$, $\Psi = \pi/200$, and $\gamma = .01$ (right). [Please format to 2 column width]

Adequate spectral directional data could not be obtained for a variety of roughness scales. Due to the oxidative nature of stainless steel 304 at high temperatures, only relative total directional emissivity data for samples of varying roughness across multiple temperatures could be found and used as a benchmark, rather than relative spectral directional. Monte Carlo sampling of wavelengths was employed to generate total directional emissivity coefficients and compared with literature values in Figure 13.

Figure 13. Total Directional Emissivity of 304 Stainless Steel. Experimental results from Rolling are shown in (a) and (c) while model output is provided in (b) and (d). [Please format to 2 column width]

Computed results for 304 stainless steel and tungsten are compared to various sources of experimental literature in figure 14 for stainless steel 304 and figure 15 for tungsten.

Figure 14. SS 304 Total Hemispherical Emissivity Coefficients from Experiment[39][46]and Model Output. [Please format to 1 column width]

Figure 15. (a) Tungsten Total Hemispherical Emissivity Coefficients from Experimental[47][48][49][50][51][52] and Model Output and (b) Zoomed-in Tungsten Total Hemispherical Emissivity Coefficients from Experimental[48][50][51] and Model Output [Please format to 1 column width]

Relatively little difference is apparent between results for case 2 (featured in figure 8) and output of case 4 (figures 14 and 15). The difference in the two results mostly comes from values at high incidence angles at the directional spectral level (which are less important due to the sin and cos terms from equations 11a and 11b).

Roughness plays a significant role in overall emissivity. In this study, it was demonstrated that a spectral directional model where roughness is physically accounted for can be sampled and iterated into generating a total hemispherical emissivity coefficient where the associated dependencies are still maintained. The surfaces used in this study were not particularly rough however the same process should be applicable to other techniques where roughness plays a greater role.

4 Discussion

It should be noted that the surface profile $f(x)$ is a unit-less, artificially-generated curve that is most likely non-representative of a real surface (such as what would be generated from a Profilometry measurement). However, by changing the Ψ parameter which determines the amplitude of $f(x)$ in the model, the model reproduces emissivity trends observed in variations of σ , a roughness parameter of real surfaces. The limitation to this method starts becoming apparent at $\Psi = \pi/10$ where small erroneous features in the directional spectral emissivity output begin to materialize. The features are most pronounced in figure 10d where the relative spectral parallelized emissivity at normal incidence starts to creep below 0.5, which should not happen. Also, noise begins appearing at around $\theta=70^\circ$ in figure 10d. Both of these features increase as Ψ increases past $\pi/10$. At rougher surfaces where this GOA adaptation loses validity, it would be necessary to implement other methods such as the direct solving of Maxwell's Equations to generate spectral directional emissivity. A different method of surface profile representation might also be desirable in such a case. However, the iterative spectral directional sampling methodology implemented here to generate total hemispherical emissivity values should be easily transferrable.

The accuracy of total hemispherical emissivity prediction is predicated on the accuracy of the input optical constants. Drude Theory appears very effective in the case of stainless steel 304 for providing the optical constants used in predicting emissivity (figure 14), but this is not case for Tungsten at very short wavelengths. As a result, the high temperature predictions of tungsten total hemispherical emissivity differ significantly from experimental literature (figure 15a). Meanwhile, lower temperature predictions maintain reasonable agreement (figure 15b).

5 Conclusion

From the spectral directional GOA, observed experimental trends of spectral directional emissivity coefficients are modeled across variations in material, wavelength, direction, roughness and temperature. While the brunt of previous modeling research has focused on spectral directional emissivity, total emissivity is obtained from the spectral directional modeling in this work. Total hemispherical emissivity values are generated from the simulation of the sampled wavelengths and reasonable agreement to experimental literature is achieved. The sampling methodology used to obtain total emissivity presented here through the GOA should be transferrable to other more-sophisticated emissivity modeling methods such as FDTD.

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