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Radiative Properties of Films Using Partial Coherence Theory

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Wave optics, geometrical optics, and partial coherence approaches for the calculation of radiative properties of single and multilayer thin films with arbitrary angles of incidence are presented with emphasis on the partial coherence approach. Solution methodologies are compared and a partial coherence approach is shown applicable over the entire range of film sizes. The effects of film thickness, angle of incidence, polarization, and bandwidth of radiation on radiative properties of single films is demonstrated. Hemispherical reflectance is used to typify gross film radiative properties over all angles. Multilayer film theory is employed to examine the effect of substrate thickness for a case of interest. Proposed regime limits are investigated using simple material models and a typical regime map delineating thick and thin films is presented.

Nomenclature

A = absorptivity
c = speed of light in vacuum
d = radiation penetration depth or skin depth
h = film thickness
Im( ) = imaginary value of complex argument
$\bar{n}$ = complex refractive index, $n + ik$
R = reflectivity
Re( ) = real value of complex argument
r = reflective coefficients
T = transmissivity
t = transmissive coefficients
x = thickness parameter, n_2h/λ_T
α = absorptance parameter using Beer's law
β = directional transmittances in the film
θ = angle of incidence or refraction
θ_2 = real angle of propagation in the film
λ = wavelength
τ = time delay
ω = angular frequency

Subscripts

g = geometrical optics
i = incident
ij = properties of the i-j interface
w = wave
$+$ = forward propagating
$-$ = backward propagating

Superscripts

0 = directly reflected/refracted fields
1 = indirectly evolved fields
* = complex conjugate
′ = reflected angle

Introduction

RADIATIVE properties of thin films or multiple layers of thin films are typically calculated using either wave or geometrical optics. The two formulations can yield dramatically different results as wave optics inherently includes the interference phenomenon important in small-scale radiative transfer. As emphasized in Wong et al.,[1] accurate modeling of thermal processes in thin films is necessary, as small changes in size can effect large changes in radiative properties. Wave optics calculates electromagnetic fields, either as time-harmonic phasors, solving for amplitude and phase, or as real time-dependent electromagnetic fields governed by Maxwell's equations. Geometric optics solutions, which are based on intensity superposition formulations and without phase considerations, cannot directly capture these wave interference scale effects. With some restrictions, geometrical optics results for thick films can be obtained by spectral integration of the wave optics solutions.[2] However, for thin films, wave interference effects change the total radiative properties of the film. Thus, some basic questions are when each formulation is most valid for thin films, and how best to describe a thin or thick film.

Tien and Chen[3] present ample motivation for the desire to discriminate between regimes while proposing limits and microscale radiation regimes. Harris et al.[4] compared the two formulations for metal films on a nonabsorbing backing and concludes that intensity superposition is applicable for metallic films with thick backings, but for some cases a wave optics formulation is necessary. Tien[5] summarized radiation in particulate systems and presented regime maps for dependent and independent scattering. Tuntomo et al.[6] considered internal absorption inside a sphere and compared the formulations. Chen and Tien[7] compare wave and geometrical optics for the case of a thin film with normal incidence and introduce a partial coherence approach to model all size ranges. Using partial coherence results they produce regime maps for nearly monochromatic incidence. Partial coherence theory is shown to describe both thin and thick limits exactly, as well as bridging the intermediate area between where neither classical method holds. Richter et al.[8] considers a partial coherence solution to single and multilayer thin films and verifies the partial coherence method with experimental results.

The objective of this study is to compare these three methods, wave, geometrical, and partial coherence optics, for the calculation of directional and hemispherical radiative properties of specularly reflecting single and multilayer films of arbitrary thickness. Partial coherence theory for arbitrary angles and multilayer films shall be presented and discussed in detail. Partial coherence theory will be shown to correctly yield total properties both in the thin and thick limits without the calculation of spectral properties and subsequent spectral integration, as is necessary for wave optics, and without the inaccuracies of geometrical optics for thin films. The concept of a time delay in partial coherence theory for non-normal incidences will be presented in detail. Reflectivity, transmis-

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sivity, and absorptivity will be calculated, and from absorptance, the emittance of the film will be obtained using Kirchoff's law. Using all three techniques, existing regime limits will be examined and a typical regime map of method validity is presented.

Analysis

We shall first consider a single homogeneous film with complex refractive index $\bar{n}_2 = n_2 + ik_2$ between two transparent dielectric media. Radiation is assumed incident at an arbitrary angle to the film θ_1 and from a remote point source. We shall restrict the film surfaces to be optically smooth and perfectly parallel. This idealization can be considered valid for cases where $\delta h << \lambda/(4n_2)$, where δh is the average departure from parallelism over the area of the beam, and the Raleigh criterion for surface roughness is met, $m < \lambda/(8 \cos \theta_1)$, where m is the height of surface irregularities.

Wave Optics

The coherent, or wave optics, formulation solves for the reflected, transmitted, and internal electromagnetic fields. Each spectral component of noncoherent incidence may be found by solving Maxwell's electromagnetic field equations using appropriate boundary conditions. Spectral reflective and transmissive coefficients at each interface, i-j, are found using the Fresnel relations and the overall reflective coefficient for the film can be found to be[9]

$$r = \frac{r_{12} + r_{23} \exp[i(2\omega/c\bar{n}_2 h \cos \theta_2)]}{1 + r_{12}r_{23} \exp[i(2\omega/c\bar{n}_2 h \cos \theta_2)]} \tag{1}$$

where formulation is dependent upon the polarization of the incident radiation. We shall find it convenient to define interfacial reflectivities and transmissivities as

$$R_{ij} = r_{ij}^* r_{ij} \quad \text{and} \quad T_{ij} = t_{ij}^* t_{ij} \tag{2}$$

The spectral reflectivity and transmissivity for a film can be found to be

$$R_w = |r|^2 = \frac{R_{12} + 2\text{Re}[r_{12}^* r_{23} \exp(2i\omega/ch\bar{n}_2 \cos \theta_2)] + R_{23} \exp\{-2[2\omega/ch \,\text{Im}(\bar{n}_2 \cos \theta_2)]\}}{1 + 2\text{Re}[r_{12}r_{23} \exp(2i\omega/ch\bar{n}_2 \cos \theta_2)] + R_{12}R_{23} \exp\{-2[2\omega/ch \,\text{Im}(\bar{n}_2 \cos \theta_2)]\}} \tag{3}$$

$$T_w = \frac{n_3 \cos \theta_3}{n_1 \cos \theta_1} \frac{T_{12}T_{23} \exp[-2\omega/ch \,\text{Im}(\bar{n}_2 \cos \theta_2)]}{1 + 2\text{Re}[r_{12}r_{23} \exp(2i\omega/ch\bar{n}_2 \cos \theta_2)] - R_{12}R_{23} \exp\{-2[2\omega/ch \,\text{Im}(\bar{n}_2 \cos \theta_2)]\}} \tag{4}$$

Unpolarized incidence properties are found as the average of the parallel and perpendicular polarizations. Total properties for the film are found by spectral integration over all wavelengths.

When size scales are very small, $(2\omega/chN_2 \cos \theta_2) << 1$, we can approximate the exponential terms in the wave formulation for reflectivity:

$$e^x \approx 1 + x \tag{5}$$

Furthermore, for the cases where absorptivity is negligible, thus "$N_2 \cos \theta_2$" is real, the reflectivity reduces to

$$R_w \approx \frac{R_{12} + 2r_{12}r_{23} + R_{23}}{1 + 2r_{12}r_{23} + R_{12}R_{23}} \tag{6}$$

which is equivalent to the interfacial reflectivity between medium 1 and medium 3 with no intermediate thin film.

Geometrical Optics

The thick film limit is solved using geometrical optics in many standard references yielding a simple and accurate solution for the total properties of thick films. Using either the ray-tracing or net-radiation method one finds film reflectivity and transmissivity as

$$R_g = R_{12} + \frac{R_{23}T_{12}T_{21}e^{-2\alpha L}}{1 - R_{21}R_{23}e^{-2\alpha L}} \tag{7}$$

$$T_g = \frac{n_3 \cos \theta_3}{n_1 \cos \theta_1} \frac{T_{12}T_{23}e^{-\alpha L}}{1 - R_{21}R_{23}e^{-2\alpha L}} \tag{8}$$

where we have assumed a Beer's law type of attenuation in the film.

Partial Coherence

Typically wave optics approaches solve for one forward and one backward propagating field in the film and track its phase. Geometrical optics ray-tracing solutions track each reflected and transmitted ray as discrete components, but do not track phase. The partial coherence model for calculation of thin film radiative properties allows for one backward and two discrete forward propagating constituents in the film (see Fig. 1), each with a phase. One field constituent is due to transmitted incident radiation E_+^0, and the other E_+^1, evolves from a reflection of the backward propagating field in the film E_- at the rear interface. Similarly, there are two components distinguished in the field reflected from the film, E_r^0 and E_r^1. The total forward propagating field inside the film is written

$$E_+(z, \theta_2) = E_+^0(z, \theta_2) + E_+^1(z, \theta_2) \tag{9}$$

Similarly, the reflected field can be written

$$E_r(z, \theta_1') = E_r^0(z, \theta_1') + E_r^1(z, \theta_1') \tag{10}$$

The two constituents are, in general, only partially coherent, as the component that evolves from the backward propagating wave has time delay τ_1 from the directly resulting components (see Fig. 2)

$$\tau_1 = 2L/(c/n_2) \tag{11}$$

where L is the optical path length in the film. The optical path in the film may be calculated as $L = h \sec \hat{\theta}_2$, where $\hat{\theta}_2$ is the real propagation angle in the medium.[10] Thus, the time delay can be written

$$\tau_1 = 2n_2 h \sec \hat{\theta}_2/c \tag{12}$$

For non-normal incidences the incident wave also has a phase-difference time delay τ_2 due to the inclination of the film

$$\tau_2 = \Delta/c \tag{13}$$

where Δ is the additional length traveled by the incident wave. The phase time delay τ_2 is due only to the angle of incidence, and can be written, upon appropriate inspection, as

$$\tau_2 = 2h \tan \hat{\theta}_2 \sin \theta_1/c \tag{14}$$

We shall further simplify the idea of time delay by combining the two time delays, Eqs. (12) and (14), to yield

$$\tau = \tau_1 - \tau_2 = 2h/c(n_2 \sec \hat{\theta}_2 - \tan \hat{\theta}_2 \sin \theta_1) \tag{15}$$

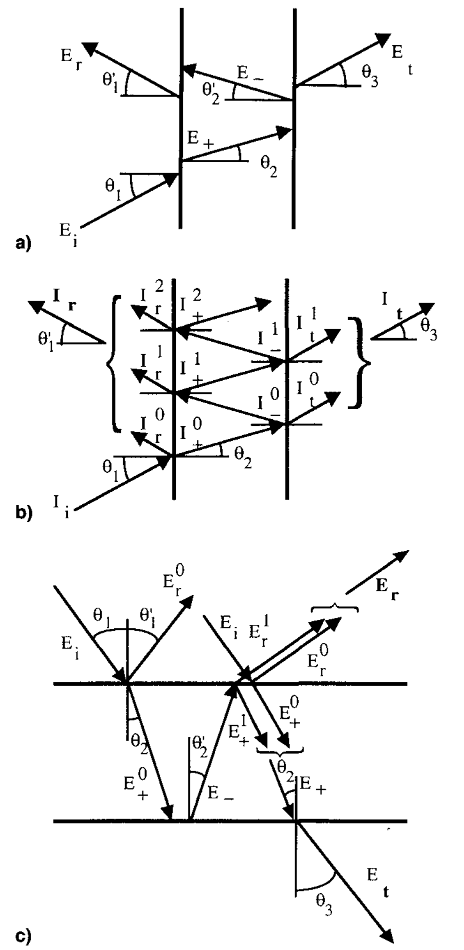

Fig. 1 Various approaches to thin film reflectivity: a) geometrical optics, b) wave optics, and c) partial coherence.

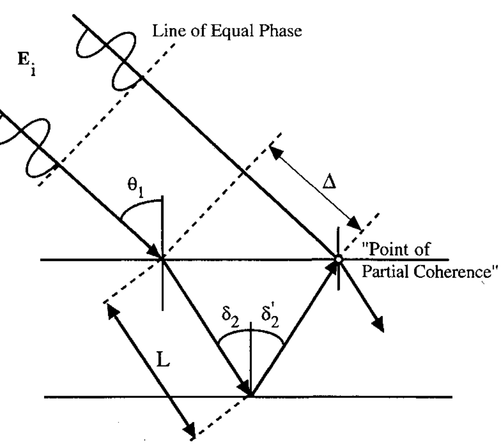

Fig. 2 Time lags in partial coherence.

The directly refracted and reflected fields can be written in terms of the incident field and the reflective and refractive coefficients for the incident, reflected, and refracted angles:

$$
\begin{aligned}
E_+^0(0, \theta_2) &= t_{12}(\theta_1, \theta_2)E_i(0, \theta_1) \\
E_r^0(0, \theta_1') &= r_{12}(\theta_1, \theta_1')E_i(0, \theta_1)
\end{aligned}
\tag{16}
$$

For monochromatic radiation, or for a nonspectrally disperse medium, r_{12} and t_{12} are given by the Fresnel coefficients and the complex refracted angle θ_2 is related by Snell's law to the incident angle θ_1. In general, due to dispersion of the optical constants, integration must be performed to get overall values of the coefficients.

The backward propagating and transmitted fields are related to the total forward propagating field by reflective and refractive coefficients for a ray incident from medium two upon medium three:

$$E_-(h, \theta_2') = r_{23}E_+(h, \theta_2) \tag{17}$$

$$E_t(h, \theta_3) = t_{23}E_+(h, \theta_2) \tag{18}$$

The evolved forward propagating and reflected field components are related to the backward propagating field

$$
\begin{aligned}
E_+^1(0, \theta_2) &= r_{21}(\theta_2', \theta_2)E_-(0, \theta_2') \\
E_r^1(0, \theta_1') &= t_{21}(\theta_2', \theta_1')E_-(0, \theta_2')
\end{aligned}
\tag{19}
$$

Inside the film, both the forward and backward field intensities are attenuated from absorption in the film. Denoting a time-average by sharp brackets, we can relate the field intensities at the film boundaries as

$$\langle E_+(h, \theta_2)E_+^*(h, \theta_2)\rangle = \beta(\theta_2)\langle E_+(0, \theta_2)E_+^*(0, \theta_2)\rangle \tag{20}$$

$$\langle E_-(0, \theta_2')E_-^*(0, \theta_2')\rangle = \beta'(\theta_2')\langle E_-(h, \theta_2')E_-^*(h, \theta_2')\rangle \tag{21}$$

where $\beta(\theta_2)$ and $\beta'(\theta_2')$ are forward and backward directional transmittances inside the film, respectively. In the case of monochromatic, or for a nonspectrally disperse medium the film transmittances may be expressed by Beer's law, $\beta = \beta' = \exp(\alpha L)$. Combining Eqs. (17), (20), and (21) gives

$$\langle E_-(0, \theta_2')E_-^*(0, \theta_2')\rangle = R_{23}\beta\beta'\langle E_+(0, \theta_2)E_+^*(0, \theta_2)\rangle \tag{22}$$

Directional transmittances and reflectances of the film are defined as

$$R(\theta_1) = \frac{\langle E_r(0, \theta_1')E_r^*(0, \theta_1')\rangle}{\langle E_i(0, \theta_1)E_i^*(0, \theta_1)\rangle} \tag{23}$$

$$T(\theta_1) = \frac{n_3 \cos \theta_3}{n_1 \cos \theta_1} \frac{\langle E_t(h, \theta_3)E_t^*(h, \theta_3)\rangle}{\langle E_i(0, \theta_1)E_i^*(0, \theta_1)\rangle} \tag{24}$$

Evaluation of Eqs. (23) and (24) requires expansion using previous field definitions. During evaluation an important term $\langle E_+(z = 0)E_-^*(z = 0)\rangle$, known as the mutual coherence function, naturally arises. When this function is normalized, it is known as the complex degree of coherence defined as[9]

$$\gamma(\tau) = \frac{\langle E_+(z = 0)E_-^*(z = 0)\rangle}{(\langle E_+(z = 0)E_+^*(z = 0)\rangle\langle E_-(z = 0)E_-^*(z = 0)\rangle)^{1/2}} \tag{25}$$

Substitution of Eqs. (18) and (20) into Eq. (24), with subsequent use of Eqs. (9), (16), (19), and (25), we calculate the directional transmittance as

$$T(\theta_1) = \frac{n_3 \cos \theta_3}{n_1 \cos \theta_1} \frac{T_{12}T_{23}\beta}{1 - 2\mathrm{Re}[r_{21}^*\gamma(\tau)](R_{23}\beta\beta')^{1/2} + R_{21}R_{23}\beta\beta'} \tag{26}$$

The directional reflectance may be evaluated by first getting an expression for the mutual coherence function, found by the substitution of Eq. (22) into the expression for coherence degree of coherence [Eq. (25)]. Multiplying Eq. (10) with its complex conjugate, substituting in Eqs. (9), (16), and (19) and taking a time average, an expression for the time-average reflected field is obtained. Substituting the resulting expressions into Eq. (23) the directional reflectance of the film is obtained as

$$R(\theta_1) = R_{12} + \left(T_{21} + 2\mathrm{Re}\left\{\frac{r_{12}t_{21}^*}{t_{12}}\left[\frac{\gamma(\tau)}{(R_{23}\beta\beta')^{1/2}} - r_{21}\right]\right\}\right) \times \frac{T_{12}R_{23}\beta\beta'}{1 - 2\mathrm{Re}[r_{21}^*\gamma(\tau)](R_{23}\beta\beta')^{1/2} + R_{21}R_{23}\beta\beta'} \quad (27)$$

Having the directional transmittance and reflectance in hand we can calculate the absorptivity, $A(\theta_1) = 1 - R(\theta_1) - T(\theta_1)$, and consequently, using Kirchoff's law, the emittance ε:

$$A(\theta_1) = 1 - R_{12} - \left[T_{23}\frac{n_3\cos\theta_3}{n_1\cos\theta_1} - R_{23}\beta'\left(T_{21} + 2\mathrm{Re}\left\{\frac{r_{12}t_{21}^*}{t_{12}}\left[\frac{\gamma(\tau)}{(R_{23}\beta\beta')^{1/2}} - r_{21}\right]\right\}\right)\right] \times \frac{T_{12}\beta}{1 - 2\mathrm{Re}[r_{21}^*\gamma(\tau)](R_{23}\beta\beta')^{1/2} + R_{21}R_{23}\beta\beta'} \quad (28)$$

Complex Coherence Function for the Coherent Limit

Absolutely coherent radiation exists only in a purely monochromatic field, although sufficiently thin films behave similarly. For a monochromatic field, the wave equation is solved, yielding exact relations between the forward and backward propagating fields as

$$E_-(0, t - \tau) = E_+(0, t)r_{23}e^{i\omega\tau} \quad (29)$$

Substitution of the previous relation into Eq. (25) yields

$$\gamma(\tau) = \frac{r_{23}^* e^{-i\omega\tau}}{(R_{23})^{1/2}} \quad (30)$$

Wave optics reflectivity [Eq. (3)] is regained after some simplifications by substituting this limiting complex degree of coherence into the partial coherence reflectance expression [Eq. (27)].

Complex Coherence Function for the Incoherent Limit

For incoherent radiation in a film, radiation is incoherent everywhere $\gamma(z) = 0$, save at the film surfaces, as discussed by Chen and Tien.[7] Radiation reflected from the surfaces has no time retardation from the incident radiation, and thus, is instantaneously coherent. In particular, at $z = h$, $E_-(h)$ is related to $E_+(h)$ and $E_+^1(z = 0)$ is related to $E_-(z = 0)$. Substitution of Eqs. (9), (16), (19), and (22) into Eq. (25) after some simplification yields

$$\gamma = r_{21}(R_{23}\beta\beta')^{1/2} + \frac{\langle E_+^0(z = 0)E_-^*(z = 0)\rangle}{(\langle E_+(z = 0)E_+^*(z = 0)\rangle\langle E_-(z = 0)E_-^*(z = 0)\rangle)^{1/2}} \quad (31)$$

Because of the time retardation τ between E_+^0 and E_- at $z = 0$, incoherence implies that the second term in Eq. (31) is zero. Thus, the expression for the complex degree of coherence between the forward and backward propagating fields at $z = 0$ simplifies to

$$\gamma(\tau) = r_{21}(R_{23}\beta\beta')^{1/2} \quad (32)$$

Assuming a Beer's law type of attenuation, substitution of this expression into Eq. (27) for directional reflectance returns the geometrical optics reflectance [Eq. (8)].

Complex Coherence Function for Partial Coherence

The complex coherence function can be separated to the form in Eq. (31) without any further assumptions on the type of radiation. Substitution of Eq. (22) into the denominator yields

$$\gamma = r_{21}(R_{23}\beta\beta')^{1/2} + (R_{23}\beta\beta')^{1/2}\frac{\langle E_+^0(z = 0)E_-^*(z = 0)\rangle}{\langle E_-(z = 0)E_-^*(z = 0)\rangle} \quad (33)$$

The mutual coherence function between two fields can be written as[9]

$$\langle E_+^0(0, t)E_-^*(0, t - \tau)\rangle = \frac{2}{\pi}\int_0^\infty G_{12}(\omega)E^{-i\omega\tau}\,d\omega \quad (34)$$

where $G_{12}(\omega)$ is known as the mutual spectral density, or cross-spectral density. It is given by

$$G_{12}(\omega) = \lim_{T\to\infty}\left[\frac{\overline{E_+^0(0, \omega)E_-^*(0, \omega)}}{2T}\right] \quad (35)$$

Solving each spectral field component using wave optics, they can be found to be

$$E_+^0(0, \omega) = t_{12}E_i \quad (36)$$

$$E_-(0, \omega) = r_{23}\exp(2i\omega/cN_2h\cos\theta_2)E_+(0, \omega) = [(r - r_{12})/t_{21}]E_i(0, \omega) \quad (37)$$

where

$$r = \left[\frac{r_{12} + r_{23}\exp(2i\omega/ch\bar{n}_2\cos\theta_2)}{1 + r_{12}r_{23}\exp(2i\omega/ch\bar{n}_2\cos\theta_2)}\right] \quad (38)$$

It is important to note that $G_{12}(\omega)$ yields a real value. Multiplication with the time-retardation gives a phase to the spectral term. Since phase is implicit in the formulations of Eqs. (36) and (37), upon substitution into Eq. (35) one drops the exponential term. Defining the incidence spectral intensity $I(\omega)$

$$I(\omega) = \lim_{T\to\infty}\left[\frac{\overline{E_i(0, \omega)E_i(0, \omega)}}{2T}\right] \quad (39)$$

we can rewrite the mutual coherence function [Eq. (34)] as

$$\langle E_+^0(0, t)E_-^*(0, t - \tau)\rangle = \frac{2}{\pi}\int_0^\infty t_{12}\left(\frac{r - r_{12}}{t_{21}}\right)^* I(\omega)\,d\omega \quad (40)$$

Substitution of the equations for fields [Eqs. (36) and (37)] into the denominator and Eq. (40) into the general equation for complex degree of coherence [Eq. (33)]

$$\gamma(\tau) = r_{21}(R_{23}\beta\beta')^{1/2} + (R_{23}\beta\beta')^{1/2}\frac{\int_0^\infty t_{12}\left(\frac{r - r_{12}}{t_{21}}\right)^* I(\omega)\,d\omega}{\int_0^\infty \left|\frac{r - r_{12}}{t_{21}}\right|^2 I(\omega)\,d\omega} \quad (41)$$

Eq. (41) is a general expression for the complex degree of coherence in a thin film. Evaluation of the integral terms in the complex degree of coherence generally requires numerical integration.

Multilayer Thin Films

Solution of multilayer thin films for both geometrical and wave optics varies little from the basic analysis of single films and is given in many references. Born and Wolf[9] give a fairly complete analysis of multilayer films using wave optics and the characteristic matrix solution method. Similarly, Siegel and Howell[10] give solution methodologies using geometrical optics. Partial coherence theory for multilayer films, as pointed out by Richter et al.,[8] may also be built up from the single film theories. Using either a recursive or matrix approach the reflectivity of the kth layer may be calculated by the single film theories set out earlier. If $\bar{r}_{k+1}$ denotes the spectral average reflectivity of the $(k + 1)$st layer and all subsequent layers and $r_{k-1,k}$, the interfacial reflectivity between the $(k - 1)$st and ith layers, then the spectrally dependent term r in the complex degree of coherence, may be calculated as

$$r_k(\omega) = \left[\frac{r_{k-1,k} + \bar{r}_{k+1}\exp(2i\omega/ch_k\tilde{n}_k\cos\theta_k)}{1 + r_{k-1,k}\bar{r}_{k+1}\exp(2i\omega/ch_k\tilde{n}_k\cos\theta_k)}\right] \tag{42}$$

If multilayer film radiative properties are to be calculated, it is important to note that film properties of the $(k + 1)$th layer, $R_{k+1}(\theta)$ and $T_{k+1}(\theta)$, are required to calculate the radiative properties of the kth layer. For the case of a single film, the necessary calculation for film reflectance was simply the interfacial reflectivity R_{23}. Thus, a simple procedure, and one used for calculation in this study, is to calculate the reflectivities recursively, starting with the rear film first. All intermediate films are then calculated until finding the reflectivity of the first film, which will then be the total multilayer reflectivity.

Calculations

Band Approximation

For reasonably monochromatic incidence, we shall approximate the spectral intensity as uniform over some band:

$$I(\omega) = \begin{cases} 1 & \omega_0 - \Delta\omega < \omega_0 < \omega_0 + \Delta\omega \\ 0 & \text{otherwise} \end{cases} \tag{43}$$

Even blackbody radiation has been quantified using an effective bandwidth.[11] Characterizing the bandwidth size is the resolution parameter f

$$f = \Delta\omega/\omega_0 \tag{44}$$

If the bandwidth is small compared with mean frequency, $\Delta\omega << \omega_0$, and thus, $f << 1$, it is reasonable to neglect dispersion effects and to use Beer's law for absorbing media. For blackbody radiation, using the concept of effective bandwidth, the resolution parameter would be above 0.41. For materials with strong emission bands, an effective bandwidth approximation could prove useful. It is also useful to define a thickness parameter x

$$x = 2n_2h\omega_0/c \tag{45}$$

We shall also handle blackbody radiation directly using numerical integration where the characteristic wavelength is given by Wien's law and emission Planck's law.

Hemispherical Reflectivity

The hemispherical reflectivity is a quantity representative of all the angular reflectivities, and therefore, provides a good measure for comparison and characterizations:

$$R_\Omega = \frac{1}{\pi}\frac{\int_\Omega R(\theta,\phi)I(\theta,\phi)\cos\theta\,d\Omega}{\int_\Omega I(\theta,\phi)\cos\theta\,d\Omega} \tag{46}$$

However, the angular dispersion of the incidence must be known. One special case useful for generalized study is the isotropic, hemispherical reflectivity defined as

$$R_\Omega = \frac{1}{\pi}\int_\Omega R(\theta)\cos\theta\,d\Omega = 2\int_0^{\pi/2} R(\theta)\cos\theta\sin\theta\,d\theta \tag{47}$$

where we also have assumed the reflectivity is independent of the polar angle ϕ. This quantity is easily calculable given angular data using a simple trapezoidal, numerical integration scheme.

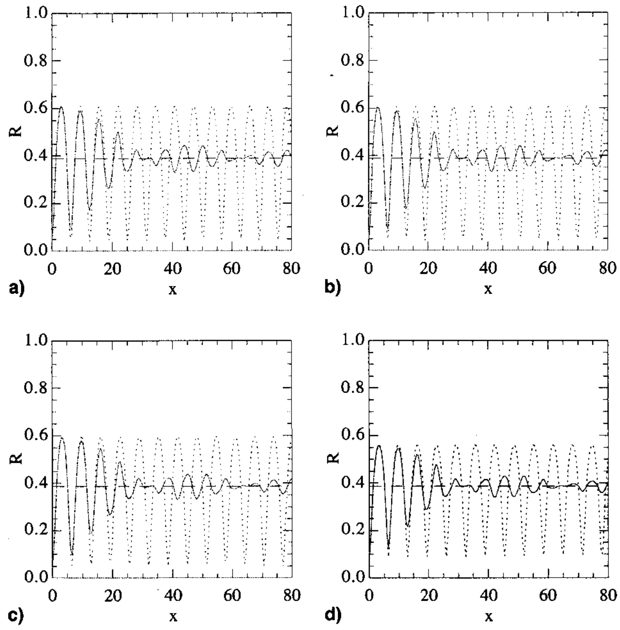

Fig. 3 Reflectivity for wave (dotted line), geometrical (dashed line), and partial coherence (solid line) approaches with thickness parameter $x = n_2h/\lambda_T \cdot \theta$ = a) 0, b) 30, c) 45, and d) 60 deg. $n_1 = 1.0$, $n_2 = 3.5$, $n_3 = 1.5$, and $f = 0.1$.

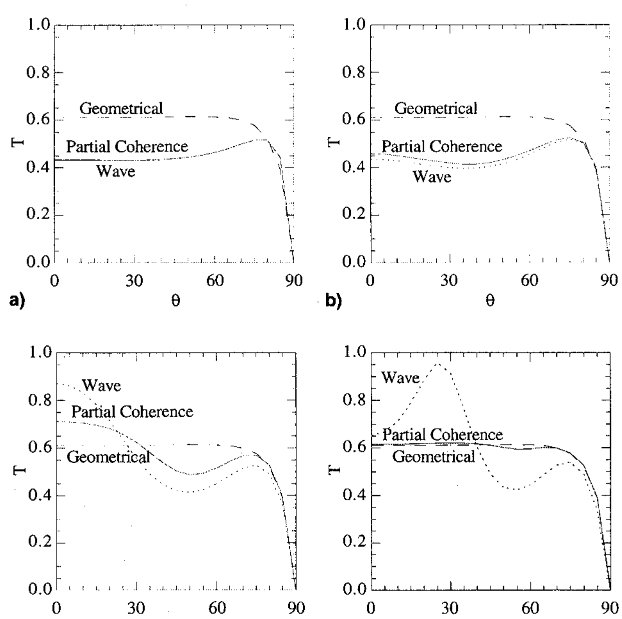

Fig. 4 Transmissivity for wave (dotted line), geometrical (dashed line), and partial coherence (solid line) approaches with incident angle. x = a) 4, b) 48, c) 100, and d) 152. $n_1 = 1.0$, $n_2 = 3.5$, $n_3 = 1.5$, and $f = 0.02$.

Results and Discussion

Some typical calculations for radiative properties are made to illustrate method limitations and the differences in the results from the three methods. In Fig. 3, reflectivity as a function of thickness for nonabsorbing films from partial coherence, wave, and geometrical optics is compared using a band approximation for nonpolarized incidence and incident angles of 0, 30, 45, and 60 deg. Notice the effect of size, as the film gets thicker partial coherence results move from the coherent solution to the geometrical optics solution with a long term periodicity related to the bandwidth. Figure 4 shows the angular dependence of transmissivity for similar films and conditions. For large angles of incidence, all solution methods yield similar results. The effect of polarization on angular reflectivity is illustrated in Fig. 5, where at large angles all methods yield similar results for each polarization. Figure 6 shows isotropic hemispherical reflectivities calculated for partial coherence with those calculated using wave and geometrical optics approaches. Reflectivity of two-film systems is studied using the multilayer partial coherence approach. Substrate thickness variation effects on radiative properties of a SiO_2/Si system are modeled. A simple, nonspectrally dependent model of the optical properties is used for both SiO_2 ($\bar{n} \approx 1.5$) and for the silicon substrate ($\bar{n} \approx 3.5 + 0.05i$). Both hemispherical and normal reflectivity values are shown in Fig. 7, emphasizing the difference in characterization between a single point value and an angular average value.

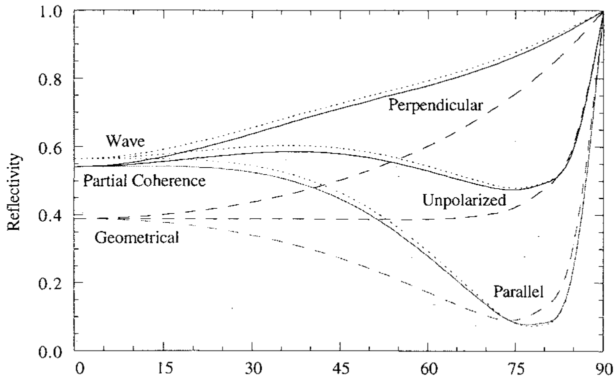

Fig. 5 Reflectivity for wave (dotted line), geometrical (dashed line), and partial coherence (solid line) approaches with incident angle for parallel, perpendicular, and unpolarized incidence. n_1 = 1.0, n_2 = 3.5, n_3 = 1.5, f = 0.02, and x = 48.

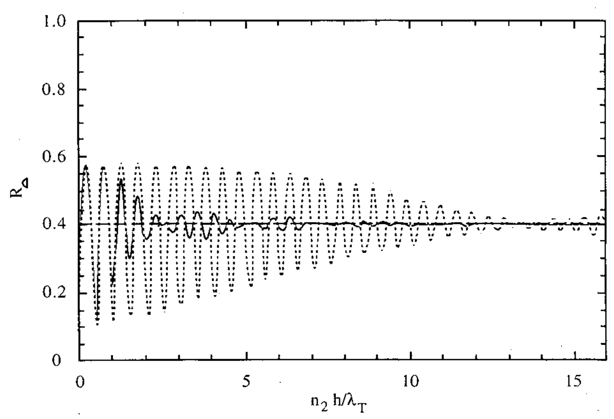

Fig. 6 Hemispherical reflectivity for wave (dotted line), geometrical (dashed line), and partial coherence (solid line) approaches with thickness parameter $x = n_2h/\lambda_T$. n_1 = 1.0, n_2 = 3.5, n_3 = 1.5, and f = 0.01.

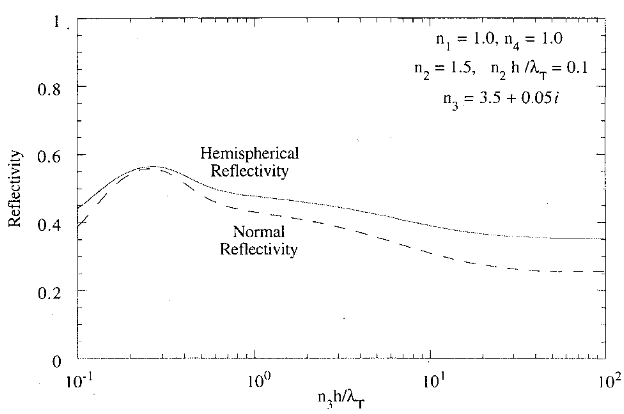

Fig. 7 Two-film reflectivity with substrate thickness variations.

Regime Maps

Chen and Tien[7] propose using the complex degree of coherence to delineate regimes where wave and geometrical optics hold, furthermore, they suggest a region where neither formulation is valid. Using partial coherence theory for normal incidence, they suggest that the wave formulation holds when $|\gamma(\tau)| \leq 0.8$ for which they find $xf = 1.13$. Also, a geometrical optics limit is recommended when $|\gamma(\tau) - \gamma_0(\tau)| \leq 0.2$, where γ_0 is the degree of coherence in the geometrical optics limit, for which they suggest: $xf = 2.59$, as a bound. Using isotropic, hemispherical reflectance as a measure of total error in radiative properties over all angles. We find that the proposed coherent limit, wave optics errors by as much as 40% in the cases studied, when compared to the partial coherence results. However, the proposed coherent limit consistently yields less than 10% error for the cases studied.

Tien and Chen[3] in their discussion of challenges in microscale heat transfer propose definitions of a first microscale radiation regime when

$$h/\lambda_T < 5 \quad \text{and} \quad d/h < 1$$

Thus, when the thickness of the film is on the same order as the characteristic free-space wavelength of the incident radiation, and the film is optically thin, they propose that wave optics solutions are appropriate. We shall examine these limits, using cases with spectral intensity approximated by blackbody emission. The characteristic free-space wavelength is the peak radiation wavelength given by Wien's law. The effect of film refractive index is examined using hemispherical reflectance in Fig. 8. This indicates a more appropriate characteristic wavelength is the peak wavelength in the film. The error for each incident angle relative to the geometrical optics solution is given in Fig. 9 for three cases. The bump in the error is due to the long range bandwidth periodicity as explained

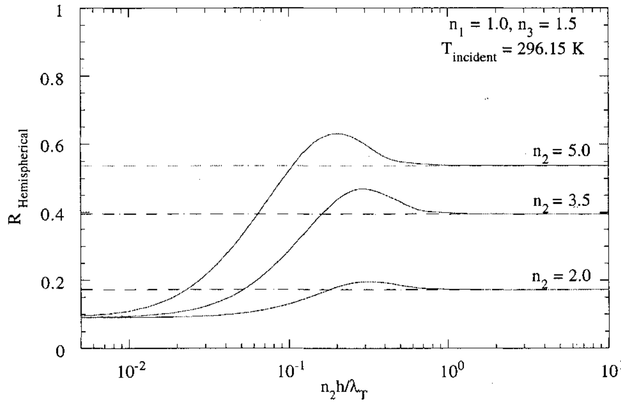

Fig. 8 Hemispherical reflectivity for geometrical (dashed line), and partial coherence (solid line) approaches with thickness parameter $x = n_2h/\lambda_T$, for three film refractive indexes.

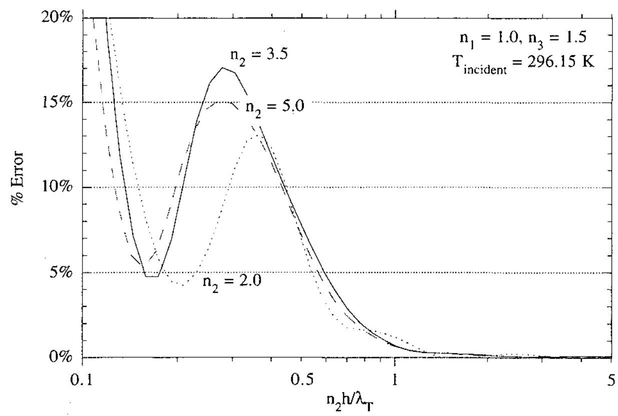

Fig. 9 Error of geometrical formulation with thickness parameter $x = n_2h/\lambda_T$ for three film refractive indexes.

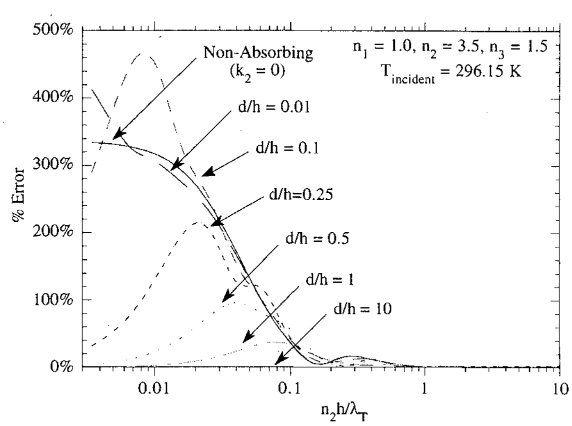

Fig. 10 Error of geometrical formulation with thickness parameter $x = n_2h/\lambda_T$ for optical thickness d/h from 0 to 10.

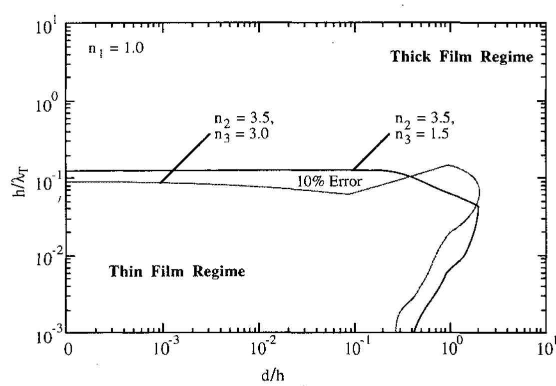

Fig. 11 Typical regime maps using blackbody radiation and hemispherical reflectance (10% error limit).

for Fig. 3. The temperature was varied to examine these bounds for three temperatures, 296, 1500, and 5780 K. For the simple cases studied, where refractive index did not vary with temperature, the reflectivity was found to be invariant with temperature.

The effect of optical thickness d/h on radiative properties was also investigated. Using a simple, spectrally gray material and blackbody incidence the optical thickness was varied from 0 to 10. Error between the calculated geometrical optics and partial coherence hemispherical reflectivities is plotted in Fig. 10 vs thickness parameter for a range of optical thickness. These plots show that geometrical optics can calculate radiative properties of optically thick $d/h > 1$ films with little error. A regime map for thickness parameter and optical thickness delineating the microscale regime based on error in hemispherical reflectivity between the geometrical and partial coherence solutions is given in Fig. 11. A 10% error in hemispherical reflectance is chosen arbitrarily as the regime boundary. The exact number is less important for regime prediction as the error slope is steep near this area, as shown in Fig. 10.

Conclusions

In an effort to clarify micro- and macroscale ranges and methodologies to describe them, three formulations for the calculation of thin film radiative properties were presented. The partial coherence formulation for arbitrary incidence angles was shown in detail and was proved to apply over all thickness ranges. Using numerical integration for the complex degree of coherence, cases were studied to demonstrate the effects of film thickness, polarization, and bandwidth of radiation on radiative properties. Gross film radiative properties for all angles were studied using the isotropic, hemispherical reflectance.

The Chen and Tien[7] regime map developed using partial coherence theory with normal incidence was investigated for arbitrary angles of incidence and a constant bandwidth spectral model. The coherent regime criteria given was found to yield errors in excess of 40% in hemispherical reflectivity. The geometrical optics, or incoherent regime criteria given were found to yield errors under 10% in hemispherical reflectivity.

Tien and Chen's[3] first microscale regime definition was investigated using simple material models with blackbody spectral incidence. It is suggested that the critical thermal wavelength is the peak radiation wavelength in the material. A regime map for thickness parameter and optical thickness is presented.

Acknowledgments

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