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Model for Alumina Nanopore-Based Optical Filter

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Alumina nanopore structures find applications in magnetic sensors, optical filters, and various biological devices. In this work, we present a ray-optics model for the optical filter. We present a detailed simulation and a simplified analytical expression for the reflectance as a function of the alumina parameters such as pore diameter, pore density, alumina thickness, and a function of the wavelength and angle of incidence of the illuminating plane electromagnetic wave. The reflectance vs wavelength in the range of 400–800 nm obtained from the simulation and the analytical expression are compared with that of the experiments for thin and thick alumina. All results agree well for a thin layer of alumina pores (90 nm). When comparing experimental and theoretical results for a thick layer of alumina (1300 nm), the results disagree. One possible explanation for the discrepancy is that the dielectric constant may vary with the thickness of the anodized alumina. Based on this work, a ray optic mixing theory is presented for waves propagating obliquely to parallel slabs of dielectric mediums with a degree of spatial periodicity.
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Physical and chemical properties of nanoscale materials depend on the geometrical shape and size.^{1–5} One of the ways to change the shape and size of the nanomaterial is to deposit them in nanopores created in anodized alumina.^{6–10} The size, density, and shape of the pores in anodized alumina can be controlled by controlling the operating voltage, current, and the electrolytic solution.^{11–13} Nanowire magnets fabricated by electrodepositing ferromagnetic alloys in anodized alumina pores have been investigated in detail for their magnetic properties.^{6–10} Commercial application of nanomagnetic-wire-based barcode has been successfully demonstrated by Choi et al.¹⁴ Antibacterial properties of silver nanowires deposited in alumina pores have been studied by Wang et al.¹⁵ Recently Chen et al.¹³ successfully demonstrated that by controlling the thickness of the alumina, for an incident white light, the wavelength of the reflected light can be controlled precisely. They were able to demonstrate that the reflected light can be tuned to the whole of the visible spectrum, thus achieving a precise optical filter using alumina film.

Saito and Miyagi^{16,17} developed a theoretical model based on a plane wave impinging on the cylindrical side of an infinite in extent cylinder based on a single isolated pore and a single row of a column of pores. A power transmissivity and a reflectivity coefficient is determined from the scattering of the wave from the column. Even though the nature of the scattered wave changes form as it propagates from one column to the next, they approximate successive scattering processes to have the same form as scattering from the first row of columns. A multiple reflection model is developed from this technique. They have theoretically predicted that when a plane wave enters the alumina at normal incidence (perpendicular to the cylindrical side of the column or row of columns) that metal-implanted alumina could be used to make an efficient polarizer with a high extinction ratio and a low insertion loss. Their work provides expressions for refractive indexes of the vertically and horizontally polarized light. Shih et al.,¹⁸ de Laet et al.,¹⁹ and Gils et al.²⁰ have used the model developed in Ref. 16 and 17 to investigate their experimental data.

Even though Chen et al.¹³ related the physics of filtering to constructive and destructive interferences of waves reflected from the top and bottom metallic surfaces, they did not elaborate on the details. The work of Saito and Miyagi^{16,17} is not applicable to oblique incidence from the cylindrical side or top of the porous alumina. That is, Brewster and internal reflection physics cannot be determined from a normal incidence study. Oblique incidence is the fundamental mechanism leading to the frequency-selective nature of the experimental work of Chen et al.¹³ In this work, we have developed a detailed model based on ray-optic physics, taking into account the geometrical shape, size, and dielectric constant of the alumina and

the pore (air). Two theoretical approaches are taken: a detailed simulation tracing the ray through the pores taking into account the refraction from each slab layer, total reflection at the base of the pore, and the initial angle of incidence and location of the white light on the surface of the nanopore film and a simplified analytical theory. In addition, based on our model, a simple mixing theory is proposed. The details of the model, including the physics and the assumptions, are presented. Results from the simulation, simple analytical theory, and experiments are presented, compared, and discussed.

Model

Snell's laws of reflection and refraction characterize the phase nature of the specular wave in diffraction and scattering theories. It is, therefore, hypothesized that the ray-optic viewpoint provides a partial picture of the wave interaction with the periodically grating thin film. It is also understood that the polarization of the wave makes a difference. That is, for a nonmagnetic medium, the Brewster angle phenomena for any two dielectrics is valid for parallel polarization but does not exist for perpendicular polarization. Because the light illuminating the film is not polarized, this phenomenon is not considered in this paper because a ray of light composed of both polarizations will always penetrate the dielectric mediums when propagating from a less optically dense medium to a more optically dense medium. Because of critical angle considerations, the reverse is not always true. If the two uniform dielectric mediums are juxtaposed in a periodic fashion with parallel interfaces, the critical angle will not be encountered as long as the ray enters the film region by way of a pore. This fact is used in the simplified ray optic model presented in the following section. The more exact ray optic theory presented next always checks for an internal reflection condition, regardless of whether the ray enters the film by way of the pore or alumina regions. In both theories, the reflected contribution of the ray at each interface inside the film is not considered because we are interested in the wave-wave interaction external to the film as a result of the transmitted ray passing diagonally through the film and reflected from the bottom surface of the film interacting with the reflected ray at the top surface of the film. It is also assumed the film is thin enough that there is a level of wave coherence among the rays reflected from the top and bottom surfaces of the film. As a result, the reflected fields add in a constructive-destructive fashion, yielding a specified frequency of illumination or color.

For a ray-optics theory to be valid, two conditions must be met in varying degrees. The surface needs to be smooth and large for ray optics to be meaningful. If the surface is rough, the reflected light will more or less be directed in all directions, yielding a diffuse reflection and transmission. This assumes that the roughness does not have a periodic pattern. The difference between diffuse and specular reflection is a matter of surface roughness; a specular re-

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Figure 1. (a) A detailed schematic figure describing the ray-optics physics pictorially. (b) The surface-reflected wave and the film-transmitted wave combining with the same angles of incidence and reflectance, yielding a constructive-destructive resultant wave at a particular frequency assuming a coherence condition is valid.

flected beam and a specular transmitted beam will be formed only if the average depth of the surface irregularities of the reflector is substantially less than a wavelength of the incident light. The second requirement for the existence of specular reflected and specular transmitted beams is that the transverse dimensions of the medium be substantially larger than the wavelength of the incident beam. If this is not the case, incident beam will be scattered in all directions with no well-defined specular beam. These claims are further supported from well-known plane-wave scattering studies from planar surfaces. For a perfectly conducting flat surface in the $z = 0$ plane, the TE^x polarization maximum of the scattered field does not occur exactly at the specular direction (specular reflection) but it approaches the value as the dimensions of the plate becomes large compared to a wavelength. The TM^x polarization maximum of the scattered field always occurs at the specular direction (specular reflection) regardless of plate size.²¹

A schematic figure showing the alumina nanopore structure and the pictorial description of the ray diagram is shown in Fig. 1a and b. In Fig. 1a, d_{po} represents the width of the pore in one dimension, which is equivalent to the diameter of a single pore in the experiment. Similarly, d_{pi} represents the width of the alumina in-between two adjacent pores. Even though the pore structure and the experiments performed by Chen et al.¹³ are three-dimensional (3D), the film is assumed to be periodically inhomogeneous in the plane of incidence and homogeneous perpendicular to the plane of incidence. Therefore, the 3D problem can be simplified to a two-dimensional problem in the plane of incidence. A thin film of Ni is electrodeposited on the top of the alumina and the base of the pore. As denoted in Fig. 1a and b, the height of the alumina film is h .

For a stationary medium at the point where the ray impinges on

an interface separating two mediums, the angle of incidence, θ_i , and angle of reflection, θ_r , are equal by Snell's law. As a ray penetrates into the film composed of nanopores, it is hypothesized that there are discrete ranges of angles of incidence relative to the film surface such that the angle of incidence that the ray makes with respect to the normal to the planar film surface upon entering the film equals the angle of refraction that the ray makes upon exiting the film at a different point in space in the region above the nanopore film surface. One might imagine that the ray upon leaving the film to the above medium is phase delayed and shifted in space, satisfying a Snell's law of reflection similar to the well-known Goos Hanchen phase shift. This implies that the angle of refraction of the ray leaving the film equals the angle of reflection of the effective phase-shifted, space-shifted ray external to the film. Even though the pore dimension is smaller than a wavelength, boundary conditions dictate that the phase of the incident, specular reflection, and specular transmission components of the wave must satisfy a phase equality condition as given by Snell's laws. It is assumed that the nanopores are nonmagnetic.

A simple analytical theory.— Assume that the total horizontal distance traveled by the ray before getting reflected from the nickel, Ni, at the bottom of the pore is $0.5l_T$. Then the relationship between l_T and h is given by

$$l_T = \frac{2h}{\tan \theta_i} \quad [1]$$

The number of pore-pillar pairs, N_p , that the ray will encounter before getting reflected is given by

$$N_p = \frac{0.5l_T}{d_{po} + d_{pi}} \quad [2]$$

The phase change incurred by the wave when traveling through one pore width and one pillar width, ϕ_{po} and ϕ_{pi} , respectively, are given by

$$\phi_{po} = 2\pi \left(\frac{d_{po}}{\cos \theta_{po}} \right) \left(\frac{1}{\lambda_{po}} \right) \quad [3]$$

$$\phi_{pi} = 2\pi \left(\frac{d_{pi}}{\cos \theta_{pi}} \right) \left(\frac{1}{\lambda_{pi}} \right) \quad [4]$$

θ_{po} and θ_{pi} are related by

$$\sqrt{\epsilon_{po}} \sin \theta_{po} = \sqrt{\epsilon_{pi}} \sin \theta_{pi} \quad [5]$$

and λ_{po} and λ_{pi} are related by

$$\lambda_{pi} = \frac{\lambda_{po}}{\sqrt{\epsilon_{pi}}} \quad [6]$$

as $\sqrt{\epsilon_{po}} = 1.0$. Using Eq. 5 and letting $\theta_{po} = \theta_i$, $\cos \theta_{pi}$ can be shown to be

$$\cos \theta_{pi} = \sqrt{\frac{\epsilon_{pi} - \sin^2 \theta_i}{\epsilon_{pi}}} \quad [7]$$

Using Fig. 1a, the angles θ_i and θ_{pi} in Eq. 7, respectively, refer to ϕ_{2j-1} and ϕ_{2j} , where $j = 1, 2, 3, \dots$. Odd values of j imply the pore opening and even values of j imply the alumina medium. Using Eq. 6 and 7, phase change in a pillar, ϕ_{pi} , can be shown to be

$$\phi_{pi} = 2\pi \left(\frac{d_{pi}}{\lambda_{po}} \right) \left(\frac{\epsilon_{pi}}{\sqrt{\epsilon_{pi} - \sin^2 \theta_i}} \right) \quad [8]$$

where λ_{po} is the wavelength of light in air. The total phase change, Φ_r , incurred by the ray which enters the alumina and gets reflected at the Ni layer at the bottom of the pore and exits from the alumina is given by

$$\Phi_t = 2N_p(\phi_{pi} + \phi_{po}) = \left(\frac{4\pi}{\lambda_{po}}\right)\left(\frac{h}{\tan \theta_i}\right)\left(\frac{1}{d_{pi} + d_{po}}\right) \times \left(\frac{d_{pi}\epsilon_{pi}}{\sqrt{\epsilon_{pi} - \sin^2 \theta_i}} + \frac{d_{po}}{\cos \theta_i}\right) \quad [9]$$

The net phase incurred by the ray reflected from the top of the alumina, Ω_t , with respect to the phase of the ray reflected at the bottom of the pore at the point of incidence is given by

$$\Omega_t = \left(\frac{4\pi}{\lambda_{po}}\right)\left(\frac{h}{\tan \theta_i}\right)\cos \theta_i \quad [10]$$

The net phase difference, Φ_n , between the rays, which reflects from the bottom of the pore and the top of the alumina, is the difference between Φ_t and Ω_t and is given by

$$\Phi_n = \Phi_t - \Omega_t = \left(\frac{4\pi}{\lambda_{po}}\right)\left(\frac{h}{\tan \theta_i}\right)\left(\frac{1}{d_{pi} + d_{po}}\right) \times \left(\frac{d_{pi}\epsilon_{pi}}{\sqrt{\epsilon_{pi} - \sin^2 \theta_i}} + \frac{d_{po}}{\cos \theta_i} - (d_{pi} + d_{po})\cos \theta_i\right) \quad [11]$$

Detailed theory and equations for simulation.—In this section, a detailed theory which traces the ray through various materials for various angles and locations of incidence on the top of the pillar is presented. The pillars or columns are treated as a one-dimensional grating. This procedure allows one to determine incident angle and location constraints where Snell's law of reflection, $\theta_i = \theta_r$ is satisfied.

The incident ray propagates at an angle θ_i relative to the tangent to the thin-film surface. If θ_o is defined as the complement angle, then

$$\theta_o + \theta_i = 90^\circ \quad [12]$$

The depth of the thin film or equivalently, the height of the column, is h . Each grating or column is defined with a region number. The ray enters column 1 of thickness D_1 and index of refraction n_1 . Each successive column the transmitted ray enters is labeled in sequential order. Therefore, the column characteristics for the m th region are n_m and D_m . Let α be a number between 0 and 1. The position of the incident ray entering the film is located a distance $\ell_1 = \alpha D_1$ from the column corner separating columns 1 and 2 and separating the thin film and the vacuum region above the thin film. The angle of the transmitted wave in medium 1 relative to the normal of the thin-film surface, θ_{T1} , based on Snell's law of refraction is

$$\theta_{T1} = \sin^{-1}\left[\frac{n_o}{n_1} \sin(90 - \theta_i)\right] = \sin^{-1}\left[\frac{n_o}{n_1} \sin(\theta_o)\right] \quad [13]$$

where n_o is the index of refraction of the medium above the thin film. For the materials of consideration, the thin film is either more optically dense (the alumina between the nanotube pores) or has the same optical density (the air region internal to the nanotube pores). If the top column is coated with a thin metal film, then a fraction of the energy will evanesce through the film and propagate into the dielectric columns. In the theory developed, this condition is avoided by adjusting the initial position of the ray relative to the film surface. Referring to Fig. 1a, the vertical distance the ray propagates in medium 1 before entering medium 2 is

$$h_1 = \ell_1 \cot \theta_{T1} \quad [14]$$

If this height is less than the column height, $h_1 < h$, then the angle the ray makes relative to the normal of the side of the column, ϕ_1 , is determined and the geometrical length of the ray, L_1 , in this medium is determined

$$\phi_1 = \pi/2 - \theta_{T1} \quad [15a]$$

$$L_1 = \ell_1 \csc(\theta_{T1}) \quad [15b]$$

If the calculated column height, h_1 , exceeds the true column height, h , then the ray is reflected on the bottom side of the film and the ray characteristics in column 1 are

$$h_1 = h \quad [16a]$$

$$\ell_1 = h \tan(\theta_{T1}) \quad [16b]$$

$$L_1 = h_1 \sec(\theta_{T1}) \quad [16c]$$

$$\theta_{B1} = \theta_{T1} \quad [16d]$$

where θ_{B1} is the angle of reflection at the bottom of the column. It is understood that reflection at the bottom of the film may be due to either a thin film of metal coating the column bottom or a result of wave evanescence between metal layers, because the column width is less than a wavelength in dimension, $D_N < \lambda$, where N signifies the N th column where reflection occurs at the bottom of the film.

Consider the m th region as the descending ray refracts from one column to the next where $m = 2, \dots, N-1$ where wave reflection occurs in the N th region. The distance parallel to the film surface, the angle of refraction into the column from the column side relative to the normal, the vertical distance, h_m , and the geometrical distance can be written as

$$\ell_m = D_m \quad [17a]$$

$$\phi_m = \sin^{-1}\left(\frac{n_{m-1}}{n_m} \sin(\phi_{m-1})\right) \quad [17b]$$

$$h_m = \ell_m \tan(\phi_m) \quad [17c]$$

$$L_m = \ell_m \sec(\phi_m) \quad [17d]$$

The condition for total internal reflection $|(n_{m-1}/n_m)\sin \phi_{m-1}| < 1$ is examined in each successive region the ray propagates. If this condition is not met, the program is terminated and a new initial ray position or initial angle of incidence is chosen. The total vertical and horizontal distances, the geometrical path length, and the optical path length the ray traverses are monitored. If the total vertical distance exceeds the height of the column, then this region is labeled as the N th region where reflection from the film bottom results.

Like the first region, the N th region is considered separately. If $N \neq 1$, then the vertical distance, h_N , the angle of refraction into the column from the column side relative to the normal, ϕ_N , the distance parallel to the film surface, ℓ_N , and the geometrical distance, L_N , are, respectively

$$h_N = h - \sum_{j=1}^{N-1} h_j \quad [18a]$$

$$\phi_N = \sin^{-1}\left(\frac{n_{N-1}}{n_N} \sin(\phi_{N-1})\right) \quad [18b]$$

$$\ell_N = h_N \cot(\phi_N) \quad [18c]$$

$$L_N = \ell_N \csc(\phi_N) \quad [18d]$$

The angle of reflection from the film bottom is $\theta_{BN} = 90^\circ - \phi_N$. The N th region is divided into two parts, ℓ_N and $\tilde{\ell}_N$. The tilde superscript signifies that the ray has been reflected from the bottom of the film in the N th region and is ascending toward the film surface. This superscript is only used in the N th region. If the reflected ray impinges on the $N+1$ region before exceeding the height of the column, then $D_N = \ell_N + \tilde{\ell}_N$. If not, then $D_N > \ell_N + \tilde{\ell}_N$. Let $\tilde{\ell}_N = D_N - \ell_N$, then $\tilde{h}_N = \tilde{\ell}_N \tan \phi_N$. If $\tilde{h}_N < h$, then the ray as it ascends enters the $N+1$ region and has the following geometrical properties

$$\tilde{\ell}_N = D_N - \ell_N \quad [19a]$$

$$\tilde{h}_N = \tilde{\ell}_N \tan(\phi_N) \quad [19b]$$

$$\tilde{L}_N = \tilde{\ell}_N \sec(\phi_N) \quad [19c]$$

If the ray exits the film through the N th column ($\tilde{h}_N > h$), then the geometrical characteristics of the ray are

$$\tilde{h}_N = h \quad [20a]$$

$$\tilde{\ell}_N = \tilde{h}_N \cot(\phi_N) \quad [20b]$$

$$\tilde{L}_N = \tilde{\ell}_N \sec(\phi_N) \quad [20c]$$

Now consider the ascending ray in the p th region beyond the N th column where wave reflection occurs. Here p is an integer greater than zero. The ray in this column does not impinge on the surface of the column, implying that $\tilde{h}_N + \sum_{j=1}^p h_{N+j} < h$. The distance parallel to the film surface, the angle of refraction into the column from the column side relative to the normal, the vertical distance, h_{N+p} , and the geometrical distance can be written as

$$\phi_{N+p} = \sin^{-1} \left[\frac{n_{N+p-1}}{n_{N+p}} \sin(\phi_{N+p-1}) \right] \quad [21a]$$

$$\ell_{N+p} = D_{N+p} \quad [21b]$$

$$h_{N+p} = \ell_{N+p} \tan \phi_{N+p} \quad [21c]$$

$$L_{N+p} = \ell_{N+p} \sec(\phi_{N+p}) \quad [21d]$$

If the critical angle is reached or exceeded while the ray ascends to the region above the film surface, the code is terminated.

Let the $N + M$ region ($p = M$) be the region where the ray exits the top surface of the thin film. If M does not equal zero, then

$$h_{N+M} = h - \left[\tilde{h}_N + \sum_{j=1}^{M-1} h_{N+j} \right] > 0 \quad [22a]$$

$$\phi_{N+M} = \sin^{-1} \left[\frac{n_{N+M-1}}{n_{N+M}} \sin(\phi_{N+M-1}) \right] \quad [22b]$$

$$\ell_{N+M} = h_{N+M} \cot(\phi_{N+M}) \quad [22c]$$

$$\theta_{TN+M} = 90^\circ - \phi_{N+M} \quad [22d]$$

$$\theta_{oN+M} = \sin^{-1} \left[\frac{n_{N+M}}{n_o} \sin(\theta_{TN+M}) \right] \quad [22e]$$

where θ_{TN+M} and θ_{oN+M} are the angles that the ray makes with the normal to the surface of the $N + M$ column internal and external to the column, respectively, upon exiting the film. The angle of reflection relative to the film surface is

$$\theta_r = 90 - \theta_{oN+M} \quad [23]$$

For the special case when $N \neq 1$ and $M = 0$, Eq. 18b, 20a-20c, 22e, and 23 hold where

$$\theta_{TN+M} = \theta_{BN+M} \quad [24]$$

For the case when $N = 1$ and $M = 0$, $h_N = \tilde{h}_N = h$, $\ell_N = \tilde{\ell}_N = h_N \tan(\theta_{T1})$, $L_N = \tilde{L}_N = h_N \sec(\theta_{T1})$, $\theta_{TN+M} = \theta_{BN+M} = \theta_{T1} = \theta_{B1}$, and Eq. 22e and 23 are valid.

The total optical path length and the relative distance along the film surface between the incident and reflected portions of the ray are, respectively

$$\ell_T = \sum_{j=1}^N \ell_j + \tilde{\ell}_N + \sum_{j=1}^M \ell_{N+j} \quad [25a]$$

$$L_T = \sum_{j=1}^N n_j L_j + \tilde{L}_N n_N + \sum_{j=1}^M L_{N+j} n_{N+j} \quad [25b]$$

Reflectance.— Incoherent light illuminates the thin film. If a longitudinal coherence condition is satisfied, then the time-averaged power is related to the square of the sum of the electric fields. Assume that the light source has a center wavelength λ with a small spectral bandwidth $\Delta\lambda$. Following a well-known time coherence treatment,²² the optical path difference (OPD) leading to a longitudinal coherence length condition occurs when

$$OPD < \frac{\lambda^2}{2\Delta\lambda} = \text{coherence length} \quad [26]$$

If the OPD is less than the coherence length, the time-averaged power is related to the square of the sum of the fields. If the OPD well exceeds the coherence length, the time-averaged power is related to the sum of the square of the fields (or sums of the powers). Partial coherence exists when the OPD approximately equals the coherence length. It is assumed that a high degree of coherence exists for the thin film and at least partial coherence exists for the thick sample. Further, it is assumed that the reflected rays, one reflected from the top surface of the film and the second ray experiencing the phase delay due to the properties of the film, have nearly the same angles of reflection. Consequently, the ratio of the time-averaged power to the time-averaged peak power is given by

$$R = \frac{P_{ave}}{P_o} = \left(\frac{1}{2} \right) \left[1 + \cos \left(\frac{2\pi}{\lambda} OPD \right) \right] \quad [27]$$

where the OPD is between two rays of the same wavelength λ . From a conservation-of-power principle, the time-averaged input power is directly related to the time-averaged peak power. Therefore, the power ratio given by Eq. 27 is equivalent to the reflectance of the medium. The reflectance is the ratio of the reflected power to the incident power.

For the simple analytical theory, the OPD is given by

$$OPD = \left(\frac{\lambda}{2\pi} \right) \Phi_n \quad [28a]$$

and for the detailed theory it is given by

$$OPD = L_T - n_o \ell_T \sin(\theta_o) = L_T - n_o \ell_T \cos(\theta_i) \quad [28b]$$

Simulation procedure.— The theory was simulated in a MATLAB environment. Special considerations were taken to examine the critical angle each time the ray propagates past an interface. If the critical angle was encountered or exceeded, the program would terminate. A thin metallic film is not accounted for on the surface of the grating. It is deduced that either the film is substantially thin or sparse that significant transmitted energy is coupled to the grating in the same manner as if the film were not present or the coupling results in those grating regions void of a metallic surface coating. When a ray at a particular initial position and angle of incidence successfully propagates through the thin film and reflects back into the region above the film, the optical path difference is examined for coherence and the angle of reflection is compared with the angle of incidence. Assuming that the index of refraction is independent of wavelength, the OPD is independent of the wavelength of the ray. Under the assumption that the index of refraction is independent of wavelength, a parameter space of initial conditions that will result in a coherent wave interaction is sought. Once obtained, Eq. 27 and 28b are used to determine what color of light can be observed at each angle of reflection.

Figure 2. (Color online) Reflectance vs wavelength for an alumina film of thickness 90 nm with incident angle 55 and 15°, (a) analytical and (b) simulation.

Results and Discussion

In our theoretical work, the following parameters are used: $d_{po} = 8$ nm; $d_{pi} = 6$ nm; and λ in the range of 400–800 nm based on the experimental work of Chen et al.¹³ The permittivity values used are $\epsilon_{pi} = 3.4 \pm 0.2$ for 55° and 2.65 for 15°. In Fig. 2a and b, reflectance (arb. units) vs wavelength (nm) for 90 nm alumina film obtained from analytical theory given by Eq. 27 and 28a is shown along with the results obtained from simulation described using Eq. 27 and 28b. In all reflectance plots, the reflectance given by Eq. 27 is doubled in order to account for the reflectance measurements greater than one obtained experimentally by Chen et al.,¹³ especially for the thick-film case. The number of minima in the reflectance vs wavelength plot and the wavelength value for which minima occurs in the experimental results of Chen et al.¹³ for incident angles of 15 and 55° agrees well with the results shown in Fig. 2. Use of variable permittivity with 25% variation over 40° range is necessary to obtain the best fit to the experimental data. Because anodization is directional, it is possible that the permittivity is anisotropic, even though there is no reported evidence of this observation. A ray diagram showing the path of the ray in and out of the film for a 55° incidence is shown in Fig. 3.

In Fig. 4a and b, reflectance (arb. units) vs wavelength (nm) for 1300 nm alumina film is obtained for incident angles of 15 and 55°. A value of 1.29 is used for the relative permittivity of alumina for both the analytical calculation and simulation based on matching the wavelength at which the first minimum occurs to that of the experimental value of Chen et al.¹³ The results of analytical theory and simulation agree very well, exhibiting similar number of maxima and minima in the reflectance value and at approximately the same

Figure 3. (Color online) A simulated ray diagram showing the path of the ray incident at 55°. The locations are in 10^{-7} cm units.

Figure 4. (Color online) Reflectance vs wavelength for an alumina film of thickness 1300 nm with incident angle 55 and 15° (a) analytical and (b) simulation.

wavelength. However, the results of our theoretical work do not even agree qualitatively with the experimental results of Chen et al.¹³ Results of Chen et al.¹³ exhibit minima for 15° at 465 and 673 nm and for 55° at 420 and 593 nm, which differs from our results shown in Fig. 4. Intuitively, one would expect many maxima and minima in the reflectance vs wavelength behavior as obtained in our theoretical work.

The discrepancy between our results and those of the experiments of Chen et al.¹³ for thicker alumina film may be due to variation in permittivity of the film with thickness of the anodized alumina. Such variations have been observed and reported in the literature²³ for anodic alumina films for thicknesses lower than used in this study. Because thicker films are in the anodic electrolytic environment for a longer time and the ions have to electrically drift larger distances through the alumina or pore, it is reasonable to expect that the stoichiometry of the alumina film may be depth-dependent. Thus, it is reasonable to expect a larger variation of stoichiometry from the top to the bottom of a thicker alumina film and hence, larger variation in the permittivity.

The other explanation for the discrepancy between the results of Fig. 4a and b and the results of Chen et al.¹³ can be attributed to possible failure of the ray-optics physics. A full diffraction theory using atomistic theory of scattering will have to be used. Even so, in the limit diffraction theory approaches a specular ray optics theory. It is not obvious such a theory will eliminate the discrepancy. Even if the theory works, it is less useful as a quick design tool for materials and optics design engineers compared to the simple analytical theory. The third possibility is that the coherence length of the light source used in the experiments by Chen et al.¹³ fails between 90 nm (thin) and 1300 nm (thick), in which case Eq. 27 is invalid because interference effects will not be present.

A mixing theory based on ray optics.—A one-dimensional mixing theory based on ray optics is developed. Ray optics is based on satisfying the phase portion of the boundary conditions at an interface leading to Snell's laws for plane or localized plane waves. The validity of ray optics was discussed in the previous section. Snell's law is based on the material characteristics of the medium under consideration. Therefore, an effective single-component dielectric medium may be determined by fitting an average ray trajectory in the effective medium to the exact trajectory in the multimaterial component medium, forcing the optical paths to be equivalent. This will provide an effective permittivity that approximates the electrical nature of the physical medium. Consider the one-dimensional, periodically grating medium above. Let the ray propagate the entire height of the column while sampling a large number of adjacent columns. The geometrical path length that the ray must traverse is then related to the end points of the ray trajectory in the original medium, $L = \sqrt{h^2 + (\sum_{j=1}^N \ell_j)^2}$. Equating the optical path length in the effective medium to the optical path length in the original medium based on the first N mediums yields

$$n_{\text{eff}} = \frac{\sum_{j=1}^N n_j \ell_j}{[h^2 + \sum_{j=1}^N \ell_j^2]^{1/2}} = [\epsilon_{\text{eff}}]^{1/2}$$

where n_{eff} and ϵ_{eff} are the effective index of refraction and effective permittivity of the modeled medium. Here it is assumed that the medium is nonmagnetic.

Conclusions

In this work, a ray-optics model for the anodized alumina based optical filter is presented. We present a detailed simulation and a simplified analytical expression for the reflectance as a function of the alumina parameters such as pore diameter, pore density, alumina thickness, and also the wavelength of the incident electromagnetic wave. The results from reflectance vs wavelength plots in the range 400–800 nm obtained from the simulation and the analytical expression are compared with those of the experiments for thin and thick alumina. All results agree well for thin alumina (90 nm), with a 25% variation in permittivity over a range of 40°, suggesting that the permittivity is anisotropic. For thick alumina (1300 nm), Chen's experimental results disagree with our theoretical study. One possible explanation for the discrepancy is that the dielectric constant may vary with the thickness of the anodized alumina. The other possibility is the possible failure of ray-optics physics for thicker films. This work suggests that more experimental work needs to be performed to measure permittivity as a function of thickness of the anodized film and also direction in the anodized alumina. Based on this work, a ray-optics-based dielectric-mixing theory is presented. The theory yields an average dielectric constant and refractive index based on the relative distances traveled by the wave through the various dielectric media.

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