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Reflection by absorbing periodically stratified media

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Abstract

Existing theory gives the optical properties of a periodically stratified medium in terms of a two by two matrix. This theory is valid also for absorbing media, because the matrix remains unimodular. The main effect of absorption is that the reflection (of either polarization) becomes independent of the number of periods N, and of the substrate properties, provided N exceeds a certain value which depends on the absorption. The s and p reflections are then given by simple formulae. The stop-band structure, which gives total reflection in bands of frequency and angle of incidence in the non-absorbing case, remains influential in weakly absorbing media, causing strong variations in reflectivity. The theory is applied to the frequency dependence of the normal-incidence reflectivity of a quarter-wave stack in which the high-index and low-index layers both absorb weakly. Analytical expressions are obtained for the frequency at which the reflectivity is maximum, the maximum reflectivity, and also for the reflectivity at the band edges of the stop band of the non-absorbing stack.

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(Some figures may appear in colour only in the online journal)

1. Introduction

Reflection by non-absorbing periodically stratified media is well understood [1–4]. Such structures reflect totally in the stop bands, which (for each of the s (TE) and p (TM) polarizations) depend on the optical parameters of the stratification. Omnidirectional reflection of both polarizations is possible within certain frequency ranges [5–7].

The purpose of this note is to examine the reflection by absorbing periodically stratified media. Stop bands no longer exist in the strict sense, but their remnants influence reflection, as we shall see. The rapid variation with angle of incidence or wavelength is smoothed by absorption. On physical grounds we expect that the strong dependence on N (the number of unit cells, or repetitions of one period of the stratification) will also be smoothed by absorption. This is shown to be true, and indeed we prove that provided N exceeds a number which is inversely proportional to the absorption, the s and p reflectivities attain a universal form, independent of N and of the properties of the substrate. In this sense, at least, reflection from an absorbing periodically stratified medium is simpler than from its non-absorbing idealization.

The idea that absorption will cause a periodically stratified medium to have the above properties is not new: early papers [8, 9] on multilayer dielectric reflectors derived asymptotic (large N) properties for the reflectance; and a recent paper on rugate filters [10] showed numerically that with absorption the reflectance approaches a limiting form as N increases, dominated by the stop-band structure. Some extensions to these results will be discussed in section 4. However, the general formulae to be derived for the reflection amplitudes of both polarizations are new, and so are some of those specific to multilayer dielectric quarter-wave stacks found in section 4.

2. Reflection of s-polarized plane waves

We use the notation and results of [4], which hold for absorbing media also, since the layer matrices giving the transmission and reflection properties of the periodic structure remain unimodular in the presence of absorption. Let the reflecting stratification contain N periods (of, for example, alternating high-index and low-index identical bilayers), and let the outer surface of the stratification be the $z = 0$ plane. Then the reflection amplitude of the s-wave is given by [4, equation (46)]

$$r_s = \frac{q_1 q_2 m_{12} + m_{21} + iq_1(m_{22} - \sigma_N) - iq_2(m_{11} - \sigma_N)}{q_1 q_2 m_{12} - m_{21} + iq_1(m_{22} - \sigma_N) + iq_2(m_{11} - \sigma_N)}. \quad (1)$$

Here $q_1 = n_1(\omega/c)\cos\theta_1$ and $q_2 = n_2(\omega/c)\cos\theta_2$ are the normal components of the incident and transmitted wavevectors (θ_1 and θ_2 are the angles of incidence and transmission) and

$$\sigma_N = \frac{\sin(N-1)\phi}{\sin N\phi} = \cos\phi - \sin\phi\cot(N\phi) \quad (2)$$

depends on the angle ϕ defined by

$$\cos\phi = \tfrac{1}{2}\text{trace } M = \tfrac{1}{2}(m_{11} + m_{22}) \quad (3)$$

where M is the 2×2 matrix of one period,

$$M = \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix}. \quad (4)$$

For example, in the special case of a high-low multilayer, consisting of N repetitions of constant refractive index n_h and thickness h followed by constant index n_ℓ and thickness ℓ, the s-wave matrix is

$$M = \begin{pmatrix} c_\ell & q_\ell^{-1}s_\ell \\ -q_\ell s_\ell & c_\ell \end{pmatrix}\begin{pmatrix} c_h & q_h^{-1}s_h \\ -q_h s_h & c_h \end{pmatrix} = \begin{pmatrix} c_\ell c_h - q_\ell^{-1}q_h s_\ell s_h & c_\ell q_h^{-1}s_h + q_\ell^{-1}s_\ell c_h \\ -q_\ell s_\ell c_h - c_\ell q_h s_h & c_\ell c_h - q_\ell s_\ell q_h^{-1}s_h \end{pmatrix}. \quad (5)$$

The wavevector normal components q_ℓ and q_h are given by

$$q_\ell^2 = \varepsilon_\ell\,\omega^2/c^2 - K^2, \quad q_h^2 = \varepsilon_h\,\omega^2/c^2 - K^2, \quad K = (\omega/c)n_1\sin\theta_1 \quad (6)$$

and we use the shorthand notation

$$c_\ell = \cos q_\ell\ell, \quad s_\ell = \sin q_\ell\ell, \quad c_h = \cos q_h h, \quad s_h = \sin q_h h. \quad (7)$$

In this case, the angle ϕ defined by (3) is given by

$$\cos\phi_s = c_\ell c_h - \tfrac{1}{2}s_\ell s_h(q_\ell^{-1}q_h + q_\ell q_h^{-1}). \quad (8)$$

For non-absorbing media, the stop bands are the regions where $\cos^2\phi > 1$.

For absorbing media, the dielectric functions ε_ℓ and ε_h are complex, related to the complex indices of refraction by $\varepsilon = \varepsilon_r + i\varepsilon_i = (n_r + in_i)^2 = n_r^2 - n_i^2 + 2in_r n_i$. Thus all of the matrix elements become complex, and ϕ (still defined by (3)) is always complex. As noted in the Introduction, we expect the reflectance to become independent of the number of periods N, if N is large enough (how large is specified below). Let $\phi = \phi_r + i\phi_i$, and assume for the moment that $\phi_i > 0$. In the definition (2) of σ_N we have

$$\cot N\phi = \frac{\cos N\phi_r\cosh N\phi_i - i\sin N\phi_r\sinh N\phi_i}{\sin N\phi_r\cosh N\phi_i + i\cos N\phi_r\sinh N\phi_i} = \frac{\cos N\phi_r(1+\xi) - i\sin N\phi_r(1-\xi)}{\sin N\phi_r(1+\xi) + i\cos N\phi_r(1-\xi)} = -i + O(\xi), \qquad \xi = e^{-2N\phi_i}. \quad (9)$$

Thus, for $N\phi_i$ large and positive, (2) and (9) give us

$$\sigma_N = \cos\phi + i\sin\phi + O(e^{-2N\phi_i}) = e^{i\phi} + O(e^{-2N\phi_i}). \quad (10)$$

If ϕ_i is negative, on the other hand, we obtain

$$\sigma_N = \cos\phi - i\sin\phi + O(e^{2N\phi_i}) = e^{-i\phi} + O(e^{2N\phi_i}). \quad (11)$$

We have thus verified our expectation that the exact number N of the stratifications becomes unimportant, provided it is large enough to make $\exp(-2N\,|\text{Im}(\phi)|)$ negligible.

Similar physical reasoning also leads us to expect that the substrate properties should become unimportant for the reflectivity, because when there is absorption and N is 'large', the incident wave does not penetrate to the substrate. Hence we expect $q_2 = n_2(\omega/c)\cos\theta_2$ to drop out of the reflection amplitude (1) at the same time as σ_N tends to its limit $\exp(\pm i\phi)$, independent of N.

What is the condition under which r_s becomes independent of q_2? Let us write the s-wave reflection amplitude as

$$r_s = \frac{\alpha q_2 + \beta}{Aq_2 + B} = \frac{\alpha(q_2 + \beta/\alpha)}{A(q_2 + B/A)}. \quad (12)$$

It will be independent of q_2 when $\beta/\alpha = B/A$, namely when

$$\frac{m_{21} + iq_1(m_{22} - \sigma)}{q_1 m_{12} - i(m_{11} - \sigma)} = \frac{-m_{21} + iq_1(m_{22} - \sigma)}{q_1 m_{12} + i(m_{11} - \sigma)}. \quad (13)$$

The condition (13) simplifies because of the unimodularity of the layer matrix $M (m_{11}m_{22} - m_{21}m_{12} = 1)$ to

$$\sigma^2 - (m_{11} + m_{22})\sigma + 1 = 0. \quad (14)$$

Since $m_{11} + m_{22} = 2\cos\phi$ from the definition (3) of ϕ, the solutions of (14) are

$$\sigma_\pm = e^{\pm i\phi} \quad (15)$$

in accord with (10), (11). The physical root of (14) is the one with modulus less than unity. We have thus obtained the result, valid when $N\,|\phi_i|$ is large, that the s-reflection amplitude takes a value independent of N and of q_2, namely

$$r_s = \frac{\alpha}{A} = \frac{q_1 m_{12} - i(m_{11} - \sigma)}{q_1 m_{12} + i(m_{11} - \sigma)} \quad (16)$$

(where σ satisfies (14)) or equivalently

$$r_s = \frac{\beta}{B} = \frac{m_{21} + iq_1(m_{22} - \sigma)}{-m_{21} + iq_1(m_{22} - \sigma)}. \quad (17)$$

3. Reflection of *p*-polarized plane waves

We can abbreviate the discussion here, because the formalism for p(TM)-polarized incidence is almost the same as for s(TE)-polarized incidence. We shall show only the differences. The p-wave reflection amplitude for an N-layer stratification is given by [4, equation (50)]

$$-r_{\mathrm{p}} = \frac{Q_1 Q_2 m_{12} + m_{21} + \mathrm{i}Q_1(m_{22} - \sigma_N) - \mathrm{i}Q_2(m_{11} - \sigma_N)}{Q_1 Q_2 m_{12} - m_{21} + \mathrm{i}Q_1(m_{22} - \sigma_N) + \mathrm{i}Q_2(m_{11} - \sigma_N)} \quad (18)$$

where

$$Q_1 = q_1/\varepsilon_1 = n_1^{-1}\left(\frac{\omega}{c}\right)\cos\theta_1,$$
$$Q_2 = q_2/\varepsilon_2 = n_2^{-1}\left(\frac{\omega}{c}\right)\cos\theta_2 \quad (19)$$

and the matrix elements m_{ij} are to be calculated as specified in section 2 of [4]. In the special case of the same high-low multilayer given as an example in section 2, the matrix for one period becomes

$$M = \begin{pmatrix} c_\ell & Q_\ell^{-1}s_\ell \\ -Q_\ell s_\ell & c_\ell \end{pmatrix}\begin{pmatrix} c_h & Q_h^{-1}s_h \\ -Q_h s_h & c_h \end{pmatrix} \quad (20)$$

where $c_\ell = \cos q_\ell \ell$, $s_\ell = \sin q_\ell \ell$, $c_h = \cos q_h h$ and $s_h = \sin q_h h$ as before. The effective wavenumbers Q_ℓ and Q_h are defined by

$$Q_\ell = \frac{q_\ell}{\varepsilon_\ell}, \qquad Q_h = \frac{q_h}{\varepsilon_h}. \quad (21)$$

The angle ϕ defined in (3) is thus given by

$$\cos\phi_{\mathrm{p}} = c_\ell c_h - \tfrac{1}{2}s_\ell s_h(Q_\ell^{-1}Q_h + Q_\ell Q_h^{-1}). \quad (22)$$

The function $\sigma_N(\phi)$, which transforms the one-period into the N-period reflection amplitude, is defined by (2) as before, but for the p-wave reflection we use ϕ_{p}, which is different from ϕ_{s} except at normal incidence. Hence we again have $\sigma_N = \exp(\pm\mathrm{i}\phi) + O(\exp(-2N\,|\phi_i|))$, and the reflection amplitude becomes independent of N for $N\,|\phi_i|$ large. Thus, by the reasoning given in the previous section, the substrate effective wavenumber component Q_2 also drops out of the reflection amplitude, which can be written in the equivalent forms

$$-r_{\mathrm{p}} = \frac{Q_1 m_{12} - \mathrm{i}(m_{11} - \sigma)}{Q_1 m_{12} + \mathrm{i}(m_{11} - \sigma)} = \frac{m_{21} + \mathrm{i}Q_1(m_{22} - \sigma)}{-m_{21} + \mathrm{i}Q_1(m_{22} - \sigma)}. \quad (23)$$

The s and p reflectivities are the absolute squares of the reflection amplitudes:

$$R_{\mathrm{s}} = |r_{\mathrm{s}}|^2, \qquad R_{\mathrm{p}} = |r_{\mathrm{p}}|^2. \quad (24)$$

We shall give an example of the application of these results in section 4.

4. Application to an absorbing quarter-wave stack

Koppelmann [8] appears to have been the first to show that weakly absorbing multilayer dielectric reflectors have limiting reflectance properties as the number of layers N increases. For a high-low stack, with refractive indices $n_h + \mathrm{i}k_h$ and $n_\ell + \mathrm{i}k_\ell$,

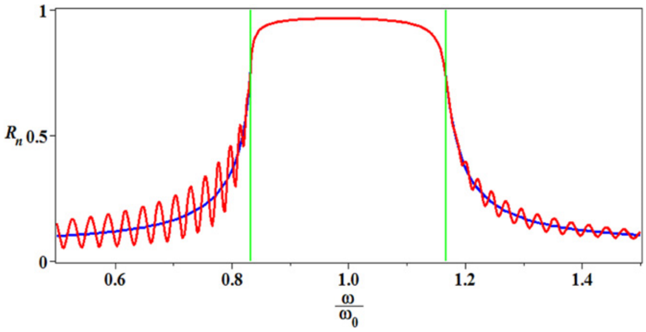

Figure 1. Normal-incidence reflectivity of a quarter-wave high–low stack, with $n_1 = 1$, $n_h = 2.35$ (ZnS), $n_\ell = 1.38$ (MgF_2) and $n_2 = 1.5$ (glass). The absorptive (imaginary) parts of the refractive indices k_h, k_ℓ have both been set to 0.01, about two orders of magnitude larger than actual values, so as to demonstrate the asymmetry in frequency dependence. The frequency range extends from $0.5\omega_0$ to $1.5\omega_0$; the stop band lies between $\omega_0 - \Delta\omega$ and $\omega_0 + \Delta\omega$, with $\Delta\omega$ given by (27). The smooth curve is the large N limit; the oscillatory curve is drawn for $N = 30$. The vertical lines indicate the limits of the stop band for an infinite non-absorbing stack.

at the design angular frequency ω_0 and quarter-wave layer thicknesses, such that

$$\omega_0/c = (\pi/2)/n_h h = (\pi/2)/n_\ell \ell, \quad (25)$$

Koppelmann showed that the reflectivity at normal incidence and at $\omega = \omega_0$ is

$$R(\omega_0) = 1 - 2\pi n_1(k_h + k_\ell)/(n_h^2 - n_\ell^2) + O(k_h^2, k_h k_\ell, k_\ell^2). \quad (26)$$

In the absence of absorption the (fundamental) stop band extends over the range $\omega_0 - \Delta\omega$ to $\omega_0 + \Delta\omega$, where

$$\Delta\omega/\omega_0 = (2/\pi)\arcsin[(n_h - n_\ell)/(n_h + n_\ell)]. \quad (27)$$

Within this range the reflectivity is unity for a non-absorbing infinite stack, and approaches unity exponentially with N [4, section 3]. The value of $\cos^2\phi$ exceeds unity: for example at $\omega = \omega_0$, $\cos\phi = -(n_h^2 + n_\ell^2)/2n_h n_\ell < -1$. Hence ϕ is complex even in the absence of absorption. Figure 1 shows the reflectance of an absorbing stack, calculated for 30 high–low layers, and also from any of the formulae (16), (17) or (23) (all equivalent at normal incidence).

The matrix elements used are as defined in (5). Over the frequency range plotted, the appropriate σ value to be used is σ_+. For example, at $\omega = \omega_0$ we find, to first order in k_h, k_ℓ,

$$\sigma_+(\omega_0) = -n_\ell/n_h + \mathrm{i}(k_h n_\ell - k_\ell n_h)/n_h^2,$$
$$\sigma_-(\omega_0) = -n_h/n_\ell - \mathrm{i}(k_h n_\ell - k_\ell n_h)/n_\ell^2. \quad (28)$$

For finite N the reflectivity is oscillatory outside of the stop-band region, $\omega_0 - \Delta\omega$ to $\omega_0 + \Delta\omega$. The oscillations increase in number and decrease in amplitude with N. Inside the stop band the difference between the finite N reflectivity and its asymptotic value is exponential in N (see section 3 of [4]), and is well below visibility in the example illustrated in figure 1.

Flannery *et al* [9] have noted that, with absorption, the maximum reflectivity is obtained at a frequency ω_m not equal to ω_0. By expanding the reflectivity obtained from (24) to first order in the imaginary parts of the refractive indices, and to second order in $\omega/\omega_0 - 1$, and differentiating the result with respect to ω, we obtain

$$\frac{\omega_m}{\omega_0} = 1 + \frac{4(k_h n_\ell - k_\ell n_h)(n_h - n_\ell)}{\pi^2[k_h(n_h^2 + 2n_\ell^2 - n_1^2) + k_\ell(2n_h^2 + n_\ell^2 - n_1^2)]} + O(k_h, k_\ell). \qquad (29)$$

To this order, the frequency shift is homogeneous of degree zero in k_h, k_ℓ. Thus even infinitesimal absorption will shift the maximum away from ω_0 by a finite amount, which seems paradoxical until one remembers that the whole range ω_0–$\Delta\omega$ to $\omega_0 + \Delta\omega$ is a maximum for zero absorption. Incidentally, the result (29) can be deduced from equation (22) of [9]. The shift will be to lower frequency, $\omega_m < \omega_0$, when $k_h n_\ell - k_\ell n_h$ is negative [$n_h > n_\ell$ is assumed]. The reflectance at $\omega = \omega_m$ is given by

$$\begin{aligned} R(\omega_m) = 1 - \{&2n_1\{\pi^2(k_h + k_\ell)[k_h(n_h^2 + 2n_\ell^2 - n_1^2) \\ &+ k_\ell(2n_h^2 + n_\ell^2 - n_1^2)] - 4(k_h n_\ell - k_\ell n_h)^2\}\} \\ &\times \{\pi(n_h^2 - n_\ell^2)[k_h(n_h^2 + 2n_\ell^2 - n_1^2) \\ &+ k_\ell(2n_h^2 + n_\ell^2 - n_1^2)]\}^{-1} + O(k_h^2, k_h k_\ell, k_\ell^2). \end{aligned} \qquad (30)$$

Another result which follows from the asymptotic (large N) formulation gives the reflectance at the band edges, $\omega = \omega_0 \pm \Delta\omega$. Again we expand in powers of k_h, k_ℓ but now fractional powers enter. (The frequencies $\omega_0 \pm \Delta\omega$ are special, forming the boundaries between different analytic parts of the zero-absorption reflectance.) As one may expect from the asymmetry expressed in (29), the reflectances are not equal. They differ from unity by terms proportional to the square root of an expression linear in the imaginary parts of the refractive indices:

$$R^\pm = 1 - \frac{n_1[(n_h + n_\ell)/(n_h - n_\ell)]^{1/2}[k_h X_h^\pm + k_\ell X_\ell^\pm]^{1/2}}{[n_h n_\ell]^{1/4}(n_h n_\ell + n_1^2)} + O(k_h, k_\ell), \qquad (31)$$

where

$$X_h^\pm = 2\pi n_\ell(n_h + n_\ell)(1 \pm \Delta\omega/\omega_0) \mp 8[n_h n_\ell^3]^{1/2} \qquad (32)$$

$$X_\ell^\pm = 2\pi n_h(n_h + n_\ell)(1 \pm \Delta\omega/\omega_0) \pm 8[n_h^3 n_\ell]^{1/2}. \qquad (33)$$

The formulae (31)–(33) are accurate to about 0.1% when the imaginary parts of the refractive indices are of order 10^{-4}, but are not useful for the much higher absorption assumed in figure 1, because of the square root dependence.

Carniglia and Apfel [11] have suggested adding layers with adjustable thicknesses, one pair at a time, in order to maximize the reflectivity. The theory presented here is restricted to periodic systems, and so cannot be applied directly to obtain analytic results in such a case.

5. Summary and discussion

We have shown that, in the presence of absorption, the exact number of layers N in the stratification disappears from the reflectivities. Likewise the properties of the substrate drop out, and one is left with simple formulae which determine the s and p reflectances. These are valid whenever N and the imaginary part of the angle ϕ (whose cosine equals half of the trace of matrix representing a single period) are such that $N\,|\mathrm{Im}(\phi)|$ is large. Even when the absorption is less than one per cent, as in the example of the previous section, the universal asymptotic formulae give the reflection properties of a finite stack of the fundamental periods, to high precision within the stop band of the non-absorbing stack, and as an average over the oscillatory reflectivity outside the stop band.

The results of sections 2 and 3 have been applied to a periodic stack of alternating uniform layers of high and low real refractive index, for which the matrix for one period can be written down exactly. The theory is however not restricted to piecewise constant dielectric functions: an arbitrary periodic dielectric function profile will have (analytically or numerically) a matrix for one period, with elements depending on the profile, frequency, angle of incidence and polarization, and the formulae derived here will give its asymptotic reflection properties.

References

[1] Born M and Wolf E 1965 *Principles of optics* 3rd edn (Oxford: Pergamon) chapter 14

[2] Yariv A and Yeh P 1984 *Optical Waves in Crystals* (New York: Wiley)

[3] Lekner J 1987 *Theory of Reflection of Electromagnetic and Particle Waves* (Berlin: Springer) chapter 12

[4] Lekner J 1994 Light in periodically stratified media *J. Opt. Soc. Am.* A **11** 2892–9

[5] Southwell W H 1999 Omnidirectional mirror design with quarter-wave dielectric stacks *Appl. Opt.* **38** 5464–7

[6] Lekner J 2000 Omnidirectional reflection by multilayer dielectric mirrors *J. Opt. A: Pure Appl. Opt.* **2** 349–52

[7] Nusinsky I and Hardy A A 2007 Omnidirectional reflection in several frequency ranges of one-dimensional photonic crystals *Appl. Opt.* **46** 3510–7

[8] Koppelmann Von G 1960 Theory of thin film layers of weakly absorbing materials and their application as interferometer mirrors *Ann. Phys.* **7** 388–96 (in German)

[9] Flannery M, Loh E and Sparks M 1979 Nearly perfect multilayer dielectric reflectors: theory *Appl. Opt.* **18** 1428–35

[10] Lakhtakia A 2011 Reflection from a semi-infinite rugate filter *J. Mod. Opt.* **58** 562–5

[11] Carniglia C and Apfel J H 1980 Maximum reflectance of multilayer dielectric mirrors in the presence of slight absorption *J. Opt. Soc. Am.* **70** 523–34