Absorption in periodic layered structures

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Abstract

Photonic band structure of metal-dielectric and semiconductor-dielectric layered structures are studied in the presence of a strong absorption. It is shown that absorption can enlarge some gaps by as much as 50%. © 2001 Elsevier Science B.V. All rights reserved.

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1. Introduction

There has been a growing interest in photonic crystals, i.e. structures with a periodically modulated dielectric constant. The latter open new ways of manipulating electromagnetic wave emission and propagation processes [1–3]. In fact, there is a common belief that, in the near future, photonic crystals systems will allow us to perform many functions with light that ordinary crystals do with electrons [3]. They also promise to become a laboratory for testing fundamental processes involving interactions of radiation with matter under novel conditions.

The basic principle behind all that is an analogy to an electron moving in a periodic potential which suggests that certain photon frequencies in a photonic crystal can also become forbidden, independent of photon polarisation and the direction of propagation — a complete photonic bandgap (CPBG). However, unlike in an ideal single-electron picture, a photon always faces the possibility of being absorbed and it is, a priori not clear if theoretical proposals for manufacturing a CPBG and which are obtained in the absence of absorption [4–8] can ever be realised experimentally. Naively, one expects that moderate absorption will only cause a slight perturbation of the band structure as confirmed in [10]. Therefore, the neglect of absorption in band structure calculations seem to be justified for purely dielectric photonic structures [14]. Unfortunately, such structures exhibit only a limited dielectric contrast which is insufficient to open a CPBG below infrared wavelengths [15–18]. A recent proposal [6–8] to obtain such a CPBG involves metallo-dielectric structures. Since metals are usually rather absorbing, this again raises the question about the effect of absorption on band structure. Here we mention in passing that systems with gain, i.e. where the imaginary part of the dielectric function ε has the opposite sign, are important for understanding laser action in new types of lasers involving photonic crystals [19].

Although the study of absorption in photonic structures is of utmost importance, so far no rigorous results exist about fundamental matters such as the meaning of band structure and band gaps for absorptive systems. Only recently, using analytic continuation techniques, it has been shown that absorption turns bands into resonances in the lower-half complex plane [20]. Literature on absorption in photonic crystals is rather sparse and, except for a recent article by Yannopapas et al. [9], only covers the cases of small absorption [10] and small filling fraction ($f_a \leq 1\%$) of the absorptive component [11–13].

2. Theory

In order to investigate numerically the effect of considerable absorption on the band structure of photonic crystals, we started with studying a one-dimensional (1D) model consisting of a periodically layered (or stratified) medium, described by the dielectric function

$$\varepsilon(\boldsymbol{x}) = \begin{cases} \varepsilon_s, & \boldsymbol{x} \in \left(na - \frac{1}{2}r_s, na + \frac{1}{2}r_s\right) \\ \varepsilon_h, & \boldsymbol{x} \notin (na - r_s, na + r_s). \end{cases} \tag{1}$$

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Here a is the lattice constant, i.e. the length of the primitive cell, n is an integer, and $r_s < a/2$. Propagation of light at normal incidence in such a stratified medium is described by the 1D periodic Helmholtz equation

$$\left[\Delta + \varepsilon(\boldsymbol{x}) \frac{\omega^2}{c^2} \right] \psi(\boldsymbol{x}) = 0, \tag{2}$$

where Δ is the Laplacian, ω the angular frequency, c the speed of light in vacuum and ψ an eigenfunction to be calculated. Another physical situation to which the 1D periodic Helmholtz equation applies (Eq. (2)) are grating-like structures [21], the so called 1D photonic crystals [22], and a number of different physical situations involving propagation of acoustic and elastic waves [23].

Below a scatterer will be a region with $\varepsilon(\boldsymbol{x}) = \varepsilon_s$ neighboured by regions with $\varepsilon(\boldsymbol{x}) = \varepsilon_h$. For notational simplicity we also set $\omega = \omega/c$. In the absence of absorption, the dispersion relation and the band structure are determined by equation, which in one dimension is identical to the Kronig–Penney equation [24]

$$s = \frac{\cos(\sigma a + \eta_0 + \eta_1)}{\cos(\eta_0 - \eta_1)} = \cos \boldsymbol{k} a, \tag{3}$$

where $\boldsymbol{k}$ is the Bloch momentum and η_l is a phase shift [25]. The latter is determined by relations

$$\cos \eta_0 = C_0 [\cos \sigma r_s \cos \rho r_s + p \sin \sigma r_s \sin \rho r_s],$$
$$\sin \eta_0 = C_0 [-\sin \sigma r_s \cos \rho r_s + p \cos \sigma r_s \sin \rho r_s],$$
$$\cos \eta_1 = C_1 [\sin \sigma r_s \sin \rho r_s + p \cos \sigma r_s \cos \rho r_s],$$
$$\sin \eta_1 = C_1 [\cos \sigma r_s \sin \rho r_s - p \sin \sigma r_s \cos \rho r_s],$$
$$C_l = \begin{cases} [1 + (p^2 - 1) \sin^2 \rho r_s]^{-1/2}, & l = 0 \\ [1 + (p^2 - 1) \cos^2 \rho r_s]^{-1/2}, & l = 1, \end{cases}$$

where $\rho = \omega \sqrt{\varepsilon_s}$, $\sigma = \omega \sqrt{\varepsilon_h}$, and $p = \sqrt{\varepsilon_s/\varepsilon_h}$ [25].

Eq. (3) still holds for absorbing scatterers but the (frequency-dependent) phase shifts η_l are now complex. Consequently, s is complex and Eq. (3) has no real eigenvalues. In accordance with [20], the eigenvalues turn into resonances in the lower complex half-plane. Some characteristic features of the complex bands of resonances can already be seen in the long-wavelength limit ($k \ll 1$), when Eq. (3) reduces to

$$\varepsilon_{eff} \, \omega^2 \approx k^2. \tag{4}$$

Here ε_{eff} is the effective dielectric constant. If we denote by f_a the absorptive material filling fraction, then

$$\varepsilon_{eff} = (1 - f_a)\varepsilon_h + f_a \varepsilon_s, \tag{5}$$

i.e. ε_{eff} is nothing but the volume averaged dielectric constant. In the long-wavelength limit, the first complex band contains an angle θ with the real positive axis which is

determined by the relation

$$\sin 2\theta = -\frac{\mathrm{Im}(\varepsilon_s)}{|\varepsilon_{eff}|} f_a. \tag{6}$$

In the limit $\mathrm{Im}(\varepsilon_s) \to \infty$, $\sin 2\theta = -1$ and hence $\theta \to -\pi/4$. For $\mathrm{Re}(\varepsilon_s) \gg \varepsilon_h$ and $\mathrm{Im}(\varepsilon_s) \gg \varepsilon_h$ one has

$$\sin 2\theta \approx -\frac{\mathrm{Im}(\varepsilon_s)}{|\varepsilon_s|} \tag{7}$$

down to such f_a that $f_a \, \mathrm{Re}(\varepsilon_s) \gg \varepsilon_h$ and $f_a \, \mathrm{Im}(\varepsilon_s) \gg \varepsilon_h$. In this range of f_a, θ exhibits only a very weak dependence on f_a.

3. Numerical results

Surprisingly enough, as shown in Fig. 1, exact numerical calculations demonstrate that the angle $\theta = \theta(\omega)$ remains very close to its value established in the long-wavelength limit often till the upper edge of the second complex band of resonances. We determined the resonances numerically for an ensemble of 1D systems with $\mathrm{Im}(\varepsilon_s)$ varied between 0 and 120 for fixed $\varepsilon_h = 1$ and $\mathrm{Re}(\varepsilon_s) = 12$. We investigated how absorption alters the relative gap width $g_w = \Delta\omega/\omega_c$, where $\Delta\omega$ and ω_c are the gap width and midgap frequency of the real part of ω, respectively. The following lessons can be learned from an investigation of the first few bands of complex resonances for a representative sample of such 1D absorptive systems.

1. If $\mathrm{Im}(\varepsilon_s)/(\mathrm{Re}(\varepsilon_s)) \leq 0.1$, the effect of absorption on the band gap is negligible (both in shifting the gap edges and in changing gap width) (see Figs. 2 and 3).
2. $\mathrm{Re}(\omega)$ ($\boldsymbol{k}$) remains a monotonically increasing (decreasing) function of the Bloch momentum for an odd (even) band (when labelled from the lowest one).
3. Absorption pushes band edges down (see Fig. 2).
4. If $\mathrm{Im}(\varepsilon_s)$ increases, the corresponding g_w tend to saturate rapidly beyond $\mathrm{Im}(\varepsilon_s) \approx \mathrm{Re}(\varepsilon_s)$ (see Fig. 3).
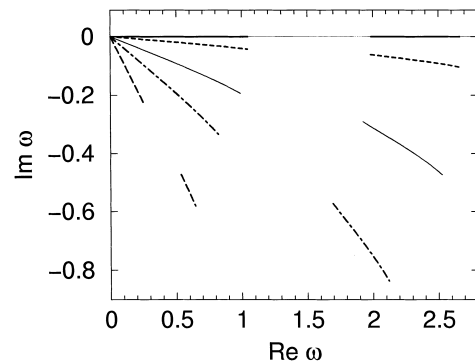

Fig. 1. When absorption is increased, bands of resonances in the complex energy plane are at larger and larger angle with respect to the real positive axis. First two complex bands are shown for absorptive filling fraction $f_a = 40\%$, $\mathrm{Re}(\varepsilon_s) = 12$, and $\varepsilon_h = 1$ as $\mathrm{Im}(\varepsilon_s)$ increases from 0 to 1, 5, 12, and 120.
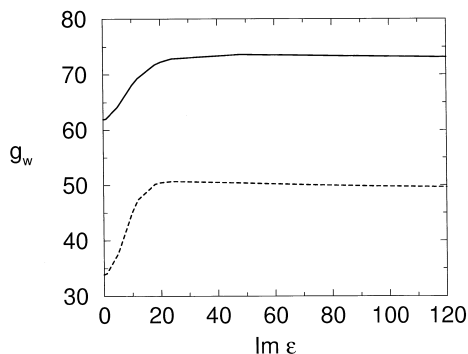
Fig. 2. As absorption increases, the band edges are pushed lower and lower. Here it is demonstrated for band edges of the real part of the first three bands of complex resonances as a function of $Im(\varepsilon_s)$. Remaining parameters are as in Fig. 1.

5. The dependence of the relative gap width g_w on $Im(\varepsilon_s)$ is monotonic up to $Im(\varepsilon_s) \approx 3 \times Re(\varepsilon_s)$ (see Fig. 3).

6. Absorption mostly increases the relative gap width g_w, although in some rare cases it can also lead to a decrease of g_w.

7. The largest effect was an increase of the g_w by 50% (see Fig. 3) and closing of the second gap which, however, reappeared again as $Im(\varepsilon_s)$ increased sufficiently enough.

8. Even if the absorptive material filling fraction f_a within the unit cell is 99% and $Im(\varepsilon_s)$ is comparable to $Re(\varepsilon_s)$, the imaginary part of the Bloch frequency eigenvalues is $\leq (Im(\varepsilon_s))/15$. Actually, it has been quite surprising to find out that the imaginary part of the frequency eigenvalues can increase when the absorptive material filling fraction within the unit cell is lowered!

It is noteworthy to say that a band gap in $Re(\omega)$ does not necessarily imply a very high reflectivity. A study of finite layered structures reveals that in the presence of a strong absorption the reflectivity at the gap centre can, for instance, saturate at 60% or less, depending on a single bilayer absorption. The latter yields a lower bound on the absorption
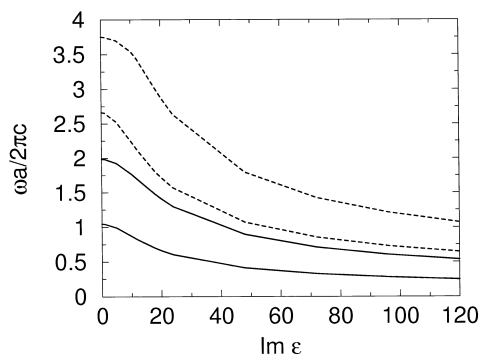
of a composite structure. The reflectivity at the gap centre is usually more than twice that for frequencies within a band, almost exclusively as a result of decreased absorption within the gap which approaches that of a single bilayer. In both cases transmissions are small. If T denotes the transmission for frequencies within a band, then the transmission within a gap is typically T^2.

A typical system to which our calculation should apply is a polymer–semiconductor or polymer–insulator layered structure where the polymer absorption dominates. Our model calculations can also apply to a semiconductor–semiconductor or semiconductor–insulator heterostructure in which one component is doped by an increasing amount of an absorptive dye. Our choice of ε_s can also be regarded as that of a metal, or an artificial metal [26], for frequencies above the plasma wavelength.

4. Conclusions

To our best knowledge, our work is the first one to deal with the case of the photonic band structure in the presence of a strong absorption, when both $Im(\varepsilon_s)$ and f_a are large $(Im(\varepsilon_s) \sim 10 \times Re(\varepsilon_s) = 120$ and $f_a \sim 99\%)$ (cf. [9–13]). Such a study of strong absorption in photonic structures is of utmost importance, both for understanding the behaviour of recently proposed metallo-dielectric structures with CPBG's below infrared wavelengths [6–8] and for new types of lasers involving photonic crystals [19]. More realistic calculations involving dispersion of the dielectric constant and including transmission and reflection properties of finite layered structures will appear elsewhere.

Fig. 3. The relative gap width of a gap in the real part of bands of complex resonances as a function of $Im(\varepsilon_s)$. Remaining parameters are as in Figs. 1 and 2.

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