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Multipole-cancellation mechanism for high-Q cavities in the absence of a complete photonic band gap

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We describe and demonstrate a new mechanism for low radiation losses in structures lacking a complete band gap, and show how resonant cavities with $Q > 10^3$ can be achieved without sacrificing strong localization in 3*d*. This involves a forced cancellation in the lowest-order term(s) of the multipole far-field radiation expansion. We focus on the system of photonic-crystal slabs, one- to two-dimensionally periodic dielectric structures of finite height with vertical index guiding. Simulations and analytical results in 2*d* and 3*d* are presented. [DOI: 10.1063/1.1375838]

Radiation losses are a general problem in many optical devices. A complete photonic band gap (PBG) prohibits losses,[1] but the difficulty of its fabrication has spurred interest in simpler 2*d*-periodic dielectric structures of finite height: photonic crystal slabs.[2–9] Without a complete gap, however, it is impossible to prevent radiation losses whenever translational symmetry is entirely broken, for example by a resonant cavity[3,7] or a waveguide bend. We introduce a mechanism[10] by which radiation losses may be minimized without an omnidirectional gap; unlike a previous, mode-delocalization mechanism,[3,7,10] we do not sacrifice localization, and operate in the interior of the gap rather than approaching a band edge. The new mechanism involves a forced cancellation of the lowest-order term(s) in a multipole expansion of the far-field radiation, distinct from the near-field multipole symmetry.

We begin by presenting the analytical foundations of this mechanism. We employ the volume–current method,[11] in which the field in a dielectric perturbation $\Delta\epsilon(\vec{x})$ is treated as a current $\vec{\mathcal{J}} = -(ik/4\pi)\Delta\epsilon(\vec{x})\vec{E}(\vec{x})$ (assuming e^{-ickt} time dependence)—then, using a Green's function $\hat{G}_\omega$, the radiated field is expressed in terms of only the field at the perturbation

$$\vec{E}(\vec{x}) = \int \hat{G}_\omega(\vec{x},\vec{x}')4\pi ik\vec{\mathcal{J}}(\vec{x}')d^3\vec{x}'. \tag{1}$$

$\Delta\epsilon$ may be chosen with respect to any structure; this determines $\hat{G}_\omega$. With $\hat{G}_\omega$ of the unperturbed crystal, one sees that the radiation can be reduced by decreasing either the perturbation or the field at the defect—delocalizing the field. Delocalization either horizontally[3] or vertically,[7] however, implies tradeoffs in device size and related issues. Instead, we focus on a new mechanism: inducing *cancellations* in the integral of Eq. (1). In particular, we study cancellations of terms in the multipole expansion of the field, using the vacuum Green's function. This $\hat{G}_\omega$ allows simple analytic study, possibly at the expense of worsened convergence—we shall see, however, that excellent convergence is still obtained with only a few multipole terms.

In the multipole method, one essentially expands Eq. (1) in terms of spherical harmonics Y_{lm}.[12] The radiated power is then an *incoherent* sum of the time-averaged power P_{lm} radiated by each multipole (proportional to the square of its multipole moment). These moments are a rapidly decreasing series, since high orders represent fast angular oscillations not present in a low-order cavity mode. Thus, if one can cancel the lowest multipole moment(s) without drastic changes in the localized field character, a large fraction of the radiated power will become zero, independent of the other moments. Such cancellations require only sign oscillations in the cavity field and degrees of freedom to control their contributions to the moment integrals. In this way, one should be able to dramatically decrease losses without sacrificing localization.

The 3*d* multipole expansion is presented in Ref. 12, and we give here the similar but simpler 2*d* expansion for transition metal (TM) fields. One finds the far-field radiation to be

$$E_z(r,\varphi) = \sum_{m=-\infty}^{\infty} a_m \frac{e^{im\varphi}}{\sqrt{2\pi}} H_m^{(1)}(kr), \tag{2}$$

where $H_m^{(1)}$ is the complex (outgoing) Bessel function. a_m is the multipole moment, determined purely from the near-field pattern

$$a_m = \frac{i\pi k^2}{2}\int J_m(kr')\frac{e^{-im\varphi'}}{\sqrt{2\pi}}\Delta\epsilon(\vec{x}')E_z(\vec{x}')d^2x', \tag{3}$$

where J_m is a Bessel function and $\Delta\epsilon = \epsilon - 1$. The time-averaged radiated power of each multipole is then $P_m = (c/4\pi^2 k)|a_m|^2$. Thus, any variation of $\Delta\epsilon$ that can lead to Eq. (3) being zero for the lowest-order a_m will minimize radiation, for which any number of root-finding procedures could be employed.

A convenient dimensionless measure of the intrinsic mode lifetime is its radiation Q.[3] We can define a Q for *each* multipole moment by a ratio of the mode energy U to the

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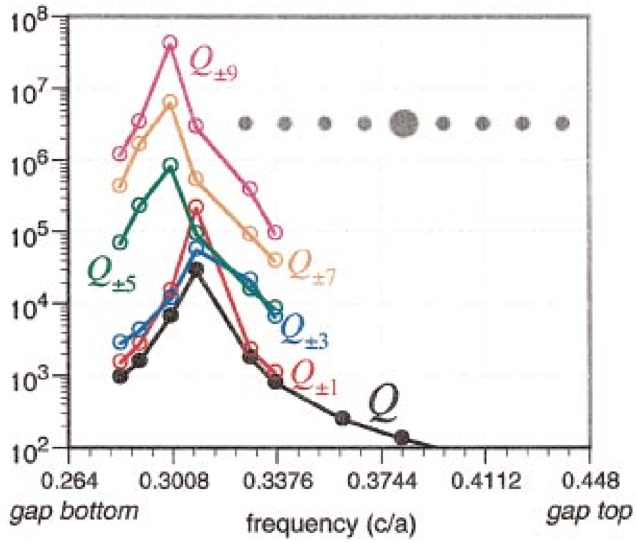

FIG. 1. (Color) Q vs ω for a dipole state in the $2d$ slab structure of the inset: a sequence of dielectric rods with lattice constant a, radius $0.2a$, and ϵ of 11.56. Both total Q (black line, filled circles) and also $Q_{\pm m}$ of the first few nonzero multipole moments (colored lines, hollow circles) are shown.

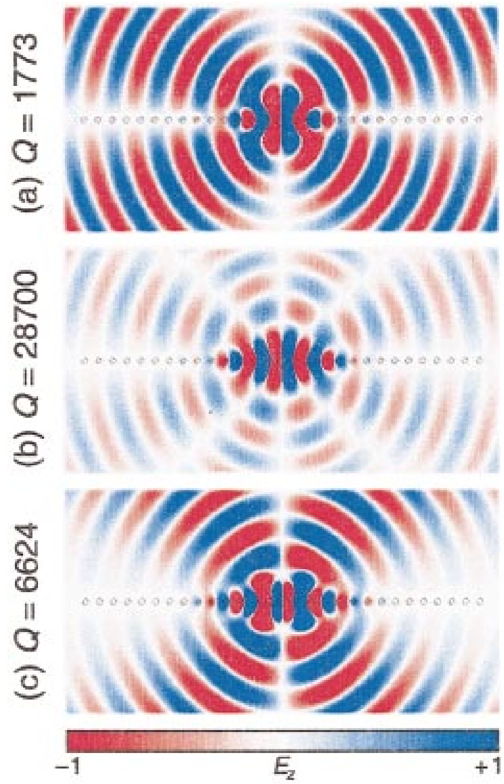

FIG. 2. (Color) E_z radiation pattern for dipole states of Fig. 1, using a color table that exaggerates small field magnitudes, with dielectric boundaries shown in black: (a) point just before the peak ($Q=1773$, $\omega=0.328$); (b) point at the peak ($Q=28700$, $\omega=0.309$) showing nodal lines from cancellation of the lowest multipole moment; (c) point just beyond the peak ($Q=6624$, $\omega=0.300$).

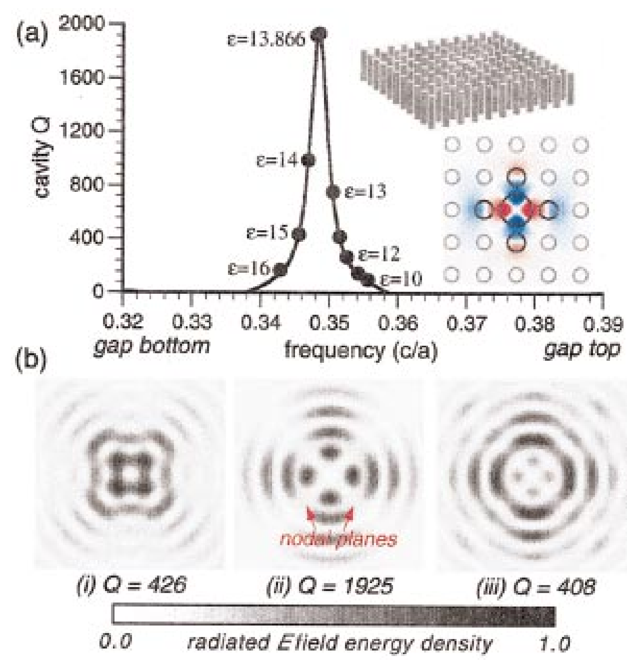

FIG. 3. (Color) (a) Q vs ω for a quadrupole state in the $3d$ slab structure of the first inset: a square lattice of dielectric rods with lattice constant a, radius $0.2a$ height $2a$, and ϵ of 12. E_z in the mid plane at peak Q is shown in the second inset. The central rod is $r=0.45a$ with $\epsilon=13$; ϵ of the four $r=0.25a$ neighbors was varied to control ω, and labels the points. The solid line is a Lorentzian curve fitted to the peak (with $R^2=0.9994$). (b) Electric-field energy density for this mode, plotted in a plane $2a$ above the rods; (i) point just before the peak ($Q=426$, $\omega=0.346$); (ii) point at the peak ($Q=1925$, $\omega=0.349$) showing nodal planes from cancellation of the lowest multipole moment; (iii) point just beyond the peak ($Q=408$, $\omega=0.352$).

radiation rate: $Q_m = ckU/P_m$.[5] Because the P_m sums incoherently, the total Q is just the inverse sum of $1/Q_m$. Although the above relations are for complex fields, they can be used for definite-frequency real fields (e.g., simulation output) via: $\mathrm{Im}\,\vec{E}=\vec{\nabla}\times\mathrm{Re}\,\vec{H}/k\epsilon$.

The above theory is general for any type of photonic-crystal system, but for definiteness we will demonstrate this phenomenon in structures involving rods in air. We will first study a simple $2d$ analogue to the photonic-crystal slab, a one-dimensional sequence of dielectric rods,[10] depicted in the inset of Fig. 1. Like the $3d$ slab, these $2d$ rods produce guided modes propagating in the lattice direction (x), with a band gap from 0.264 to 0.448 c/a, which are confined in the transverse (y) direction by index guiding (a is the lattice constant). Here, we only consider TM-polarized light (electric field along z). Next, the $3d$ system that we will examine is a square lattice of short dielectric rods in air, shown in the Fig. 3 inset. This $3d$ structure is analyzed in Ref. 6 and exhibits perfectly guided modes (extended in the slab and localized vertically). There is a band gap in the guided modes of odd symmetry with respect to the horizontal mirror plane, corresponding to TM modes in $2d$.

To study resonant cavities, we use $2d$ and $3d$ finite-difference time-domain (FDTD) calculations with absorbing boundary conditions.[13] The computational cell contains 29 rods in $2d$ and 11×11 lattice rods in $3d$, with the defect(s) at the center. The resolution is 20 pixels/a in $2d$ and 10 pixels/a in $3d$. The $3d$ TM-like gap was found to be 0.320–0.391 c/a, using a single-rod FDTD calculation with Bloch-periodic xy boundaries. Cavity modes are excited by dipole sources arranged in the same symmetry as the mode of interest, and from the field as a function of time in the cavity, the mode frequencies and decay constants (whence Q) are extracted by the filter-diagonalization method with a Fourier basis.[14]

In the $2d$ system, we form a dipole-mode defect by increasing the radius of a single-rod, pulling a single mode down into the gap.[10] The resulting Q versus frequency for a range of radii is shown in Fig. 1, along with its Q_m decomposition. Q exhibits a sharp peak of almost 3×10^4 in the interior of the gap. In contrast, the delocalization mechanism for high Q leads to a Q divergence towards a band edge. To verify that the peak in Q comes from multipole cancellation, one need only look at the radiation pattern, shown in Fig. 2: at the peak Q, extra nodal lines appear, proving that the radiation pattern of Eq. (2) has transitioned to a higher order. Quantitatively, the computed Q_m are shown in Fig. 1, and the lowest multipole moment dominates everywhere *except* at the peak, where the next moment supercedes it. The expansion converges since the Q_m increase rapidly with m. (The close-set peaks in the higher moments may suggest that a more compact representation could be found, e.g., using the crystal Green's function.) By symmetry, even multipole moments are zero and are not shown, and we have combined Q_m and the equal Q_{-m} into $Q_{\pm m}\equiv(Q_m^{-1}+Q_{-m}^{-1})^{-1}$. The total Q computed by combining these Q_m terms is within 4% of the Q measured from the field decay.

An example of the same effect in the 3d crystal occurs with a (nondegenerate) quadrupole state produced by increasing the radius of a rod to 0.45a and its ϵ to 13. We also increased the radii of the four adjacent rods to 0.25a and varied their dielectric constants to adjust the mode frequency. [The simultaneous variation of ϵ and radii was due to the limited computational resolution; in a real system, radii alone (or other geometric parameters) would be sufficient.] The resulting Q, shown in Fig. 3(a), again displays a sharp peak (of almost 2000) in the gap interior. To verify that this is due to multipole cancellation, we plot in Fig. 3(b) the radiated energy density just below, at, and above the peak ω. Two clear nodal planes appear precisely at the peak, indicating the cancellation of the lowest-order multipole moment. (The near-field patterns are visually indistinguishable in the three cases.) Similar peaking of Q in the gap interior (at more than 10^4) was reported in a photonic-crystal slab of holes,[5] and we suspect that the explanation there must also be a multipole cancellation; this is under investigation.

In summary, we have introduced a general mechanism for high-Q resonant cavities without a complete PBG, based on forced cancellation of the lowest-order multipole moment(s), that does not sacrifice localization. It could be applicable to a wide variety of optical cavities, and even combined with mode delocalization. The signature of this mechanism is that the far-field multipole character is distinct from that of the near field at a peak Q in the gap interior.

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