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Photonic bound states in periodic dielectric materials

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It is demonstrated that lattice imperfections in a periodic array of dielectric material can give rise to fully localized electromagnetic states. Calculations are performed by using a plane-wave expansion to solve Maxwell's equations. The frequency of these localized states is tunable by varying the size of the defect. Potential device applications in the microwave and millimeter-wave regime are proposed.

Recently, it has been suggested that a dielectric material with a three-dimensional periodicity may have a "photonic gap" in its frequency spectrum in which *propagating* electromagnetic modes are forbidden.[1] It has also been proposed that photonic states in this forbidden region should be localized in all three dimensions.[2] Calculations by Ho, Chan, and Soukoulis have shown that a diamond lattice of dielectric spheres can indeed have such a gap.[3] In this paper, we show that lattice imperfections can introduce exponentially localized states in the photonic band gap. We focus on the frequency spectrum of dielectric structures containing defects in an otherwise perfect diamond lattice. In our calculations, we consider impurities of two types, air spheres in the dielectric region and dielectric spheres in the air region. In both cases, localized photon modes are found to be introduced into the gap. Variation of the size of the impurity sphere leads to complete tunability of the frequency of this localized mode.

Although localized modes are common in metallic cavities, these photonic bound states are unique and physically interesting because they are localized in an entirely dielectric medium. Moreover, they have discrete frequency spectra and may be constructed from low-loss dielectric materials. Therefore, it may be possible to reduce the dissipation inherent in metallic cavities, due to skin heating of the metallic walls, and produce discrete modes with long lifetimes and correspondingly sharp frequency resonances. We propose that this effect can be exploited to produce high-quality resonant cavities and filters in the microwave and millimeter-wave regime.

In order to calculate the electromagnetic frequency spectrum of dielectric lattices, a number of authors[3–5] have suggested expanding the electromagnetic fields in a plane-wave basis,

$$\mathbf{H}(\mathbf{r})=\sum_{\mathbf{G}}\sum_{\lambda=1,2} h_{\mathbf{G},\lambda}\hat{\boldsymbol{\epsilon}}_{\lambda}e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}}, \tag{1}$$

where $\mathbf{k}$ is in the Brillouin zone, $\mathbf{G}$ is summed over the reciprocal lattice, and $\hat{\boldsymbol{\epsilon}}_{\lambda}$ are orthogonal to $(\mathbf{k}+\mathbf{G})$. Maxwell's equations are then expressed as a simple eigenvalue equation,[3]

$$\sum_{\mathbf{G}',\lambda'} H^{\lambda,\lambda'}_{\mathbf{G},\mathbf{G}'}h_{\mathbf{G}',\lambda'}=\omega^2 h_{\mathbf{G},\lambda}, \tag{2}$$

where $c=1$ and

$$H_{\mathbf{G},\mathbf{G}'}=|\mathbf{k}+\mathbf{G}||\mathbf{k}+\mathbf{G}'|\epsilon^{-1}_{\mathbf{G},\mathbf{G}'}\begin{pmatrix}\hat{\boldsymbol{\epsilon}}_2\cdot\hat{\boldsymbol{\epsilon}}_{2'}, & -\hat{\boldsymbol{\epsilon}}_2\cdot\hat{\boldsymbol{\epsilon}}_{1'}\\ -\hat{\boldsymbol{\epsilon}}_1\cdot\hat{\boldsymbol{\epsilon}}_{2'}, & \hat{\boldsymbol{\epsilon}}_1\cdot\hat{\boldsymbol{\epsilon}}_{1'}\end{pmatrix}, \tag{3}$$

and $\epsilon^{-1}_{\mathbf{G},\mathbf{G}'}$ is the Fourier transform of the inverse of the dielectric function $\epsilon(\mathbf{r})$. This eigenvalue equation is then solved to yield the normal mode coefficients and frequencies of the electromagnetic modes. Having solved for $\mathbf{H}(\mathbf{r})$, the other electromagnetic fields can be determined simply. This technique provides a simple and powerful method to solve problems in electrodynamics which takes full account of the vector nature of the electromagnetic radiation. The approximations, the finite size of the plane-wave basis and Fourier transform grid, can both be improved systematically.

Of the three similar techniques discussed in Refs. 3–5, we chose to employ the methods of Ho, Chan, and Soukoulis.[3] First, they Fourier expand $\mathbf{H}(\mathbf{r})$ rather than $\mathbf{E}(\mathbf{r})$ or $\mathbf{D}(\mathbf{r})$. Since $\mathbf{E}(\mathbf{r})$ and $\mathbf{D}(\mathbf{r})$ are discontinuous at interfaces between media with differing dielectric constants, but $\mathbf{H}(\mathbf{r})$ is continuous (with discontinuities in its first derivatives), we expect $\mathbf{H}(\mathbf{r})$ to have faster plane-wave convergence. Second, Ho, Chan, and Soukoulis[3] expand $\mathbf{H}(\mathbf{r})$ in a basis of transverse plane waves, rather than expanding in a complete basis, solving for the normal modes, and then projecting out the longitudinal solutions.

Although we would like to study the effect of a single defect in an otherwise perfect lattice, computationally it is desirable to choose a system with a finite unit-cell size. Therefore, we employ the supercell method in which we place one defect in a repeated cell of atoms. In our calculations, we used the 8-atom conventional cell of diamond.

We have performed tests using larger supercells containing 16 and 32 atoms and found similar results. We also considered supercells of 2, 4, 8, and 16 atoms containing dense impurities in the (111) planes, in order to determine the dependence of bandwidth on impurity separation. We expand in plane waves up to a finite frequency, including ~ 130 plane waves per polarization, per primitive unit cell. Based on our calculations of a one-dimensional system of periodic dielectric slabs, for which an exact solution is available,[6] we expect that the frequencies are correct to within $\sim 5\%$ at this plane-wave cutoff. Although fully converged calculations in these one-dimensional systems agreed to 0.1% we found that convergence in absolute frequencies was relatively slow in comparison to conventional electronic-structure calculations. We attribute this to the discontinuity in the first derivative of $\mathbf{H}(\mathbf{r})$ at the dielectric surfaces. In order to calculate the density of states $D(\omega)$, we sampled the frequencies at 48 k points in the irreducible Brillouin zone of the 8-atom unit cell, and then coarse grained the resulting frequencies. Although we have checked explicitly that $\omega(\mathbf{k}) = vk$ at long wavelengths and therefore $D(\omega) \propto \omega^2$, this is not accurately represented in $D(\omega)$ because of our coarse sampling of the Brillouin zone.

Since the existence of a photonic gap is a prerequisite for the existence of photonic bound states, we chose to begin our search for localized modes considering a diamond structure with a large gap to midgap ratio. Following the results of Ho, Chan, and Soukoulis,[3] we considered the periodic arrangement of spheres of air in a dielectric medium. We considered a material with dielectric constant of 35, and chose air spheres of radius $0.29a$ where a is the conventional lattice constant of the diamond cell. We considered impurities of two types, air spheres in the dielectric region, which were located at the hexagonal site,[7] and dielectric spheres in the air region, which were located in the bond-center site.[7] We also studied a diamond lattice of dielectric spheres in air, and found evidence for photonic bound states when an air sphere was placed at the bond-center site.

Since the applicability of a band structure breaks down when an impurity destroys the translational symmetry of the dielectric lattice, we have calculated the density of states of the impurity system. The density of states of the bulk diamond lattice and of diamond with a single impurity are shown in Fig. 1. As in Ref. 3, we see that the perfect diamond crystal has a gap in its photonic band structure. Placing an air sphere at the hexagonal site introduces a single state in the gap, at ω_b. Since there are no traveling modes in the diamond lattice at ω_b this must be a localized mode. This is verified in Fig. 2, which shows that the field is localized about the defect. In fact, we find that bound states whose frequencies are in the center of the gap have decay lengths as small as one lattice constant. We expect that this length will diverge as the bound-state frequency approaches the continuum of extended states.

In Fig. 1 it appears that the localized modes are spread over a modest range of frequencies. This is purely an artifact of our supercell technique. Because we are considering an array of defect states each of which is localized over some finite distance, there is tunneling between localized states on neighboring impurities. It is this hopping between defect states that introduces a nonzero width to the impurity band. For simplicity, we chose the maximum of the defect density of states to identify the actual position of the impurity state. In the inset of Fig. 1, we show calculations of the bandwidth for increasing impurity separations. This bandwidth decreases exponentially, as expected for exponentially bound states. Of course, in an experiment the lattice will be of finite size, and so the impurity mode will have some exponentially small amplitude at the walls of the lattice. This will allow the localized state to tunnel out, and will introduce a finite width to the frequency spectrum.

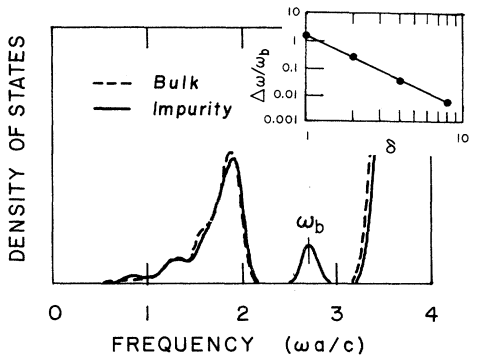

FIG. 1. Density of states in ideal diamond lattice (dashed line), and diamond lattice with defect of radius $0.15a$ located at hexagonal site (solid line). Ideal diamond lattice has a gap in the density of states in which there are no propagating modes. The defect introduces a single localized state in this gap at ω_b. Inset shows the bandwidth $\Delta\omega$ normal to a plane of impurities as a function of the (111) impurity plane separation, δ. Note that the bandwidth is exponential in the impurity separation, as expected for exponentially bound states. Units of frequency are $2\pi/a$, where a is lattice constant of the conventional unit cell, and $c = 1$.

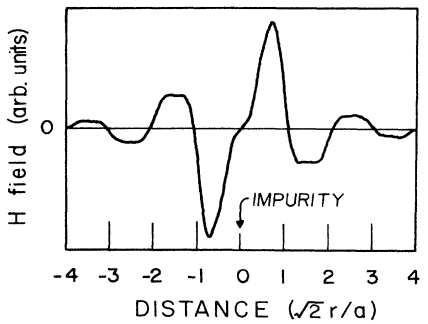

FIG. 2. **H** field associated with the state localized about a defect at the hexagonal site. $\mathbf{H}(\mathbf{r})$ is plotted along an axis which passes through the impurity at $r = 0$, and extends in the [110] direction. Because of a mirror symmetry through the $(1\bar{1}0)$ plane, $\mathbf{H}(\mathbf{r})$ lies in the $[1\bar{1}0]$ direction. Note that the localized state shows exponential decay with the sign alternating between neighboring cells.

Qualitatively, we can understand this result by analogy with the more familiar case of impurities in a crystal with a band gap in its electronic structure. Since the wavelength of light is shorter in the dielectric, these regions are analogous to a region of deep potential in the crystal. Inserting a dielectric impurity adds an attractive potential. Sufficiently strong potentials can pull a state out of the photonic conduction band into the gap, and increasing the attractive character decreases the bound-state frequency, see Fig. 3. Similarly, adding an air sphere to the dielectric region is analogous to adding a repulsive potential which pushes a state out of the photonic valence band. In fact, the addition of an air sphere defect to the perfect diamond lattice decreased the number of valence states by one, and it created one state in the gap. We found one notable difference between air and dielectric impurities. While the presence of an air sphere creates a single, well-defined state in the gap, the presence of a dielectric sphere introduces a number of states in the gap, the lowest of which is doubly degenerate and is represented in Fig. 3.

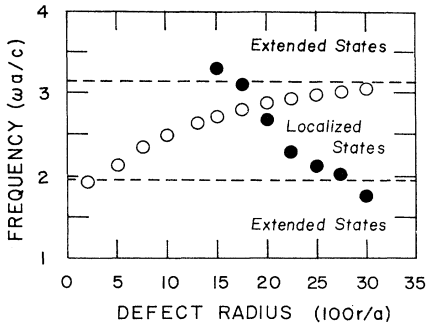

FIG. 3. Frequencies of localized modes due to lattice defects as a function of defect size. Open circles show frequencies of air spheres at the hexagonal site, and solid circles show frequencies of dielectric spheres at bond-centered sites. The dashed lines separate the regions of extended and localized states. The radius of the defect is in units of $a/100$ and the frequencies are in units of $2\pi/a$, where a is the lattice constant of the conventional unit cell, and $c=1$.

Alternately, one can understand the localized mode as a three-dimensional Fabry-Pérot interferometer.[2] Since there are no propagating modes in the dielectric material with frequencies in the gap, it behaves as a mirror to these frequencies. The defect, then, is surrounded by reflecting walls, and the localized state is analogous to the familiar resonances of a metallic cavity.

We have also considered potential microwave and millimeter-wave device applications for periodic dielectric materials as resonant cavities and filters.

Materials with high dielectric constant are currently used to fabricate resonant cavities at microwave and millimeter-wave frequencies.[8] Dielectric cavities reduce the size and cost of microwave and millimeter-wave circuits by replacing bulky discrete metallic waveguides and cavities with planar technology amenable to integrated circuit fabrication. However, all planar circuits require metallic shielding in order to reduce radiation losses and to control higher-order cavity modes. Since the fields attenuate only as $1/r$ from a typical dielectric cavity, conduction losses due to the shielding can be appreciable. Embedding these dielectrics in a lattice will reduce these losses, since the field attenuates exponentially in the lattice region.

Because of the strong localization in these lattices, it seems likely that impurities in dielectric lattices will have less power dissipation than a well-polished metallic cavity. If the power dissipation indeed turns out to be less, then dielectric lattices would certainly be valuable as high-Q resonant cavities. Even if the power dissipation turns out to be greater, there are still advantages. As one attempts to work at higher wavelengths, the small size of a metallic cavity reduces the device power rating to levels that are too small for many applications. It may be possible to store larger electric fields in dielectric lattices without burning out the device.

A second potential application for periodic dielectric materials exploits the narrow linewidth of the forbidden state in a manner similar to a Fabry-Pérot interferometer. Since a narrow transmission gap exists for all orientations, there are no collimation losses. Second, it may be possible to tune the filter by moving the impurity within the dielectric lattice.

In conclusion, we have performed calculations of the density of states of dielectric lattices containing defects. We find that defects can introduce localized modes, whose frequencies lie in the photonic band gap. We have studied size dependence of two types of defects, air spheres in dielectric and dielectric spheres in air. Finally, we have outlined potential device applications for localized modes in dielectric lattices.

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