

Numerical analysis of eigenmodes localized at line defects in photonic lattices

Kazuaki Sakoda

Research Institute for Electronic Science, Hokkaido University, Kita-ku, Sapporo 060, Japan

Tsuyoshi Ueta and Kazuo Ohtaka

Department of Applied Physics, Faculty of Engineering, Chiba University, Yayoi-cho, Inage-ku, Chiba 263, Japan

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We calculated the eigenfrequencies and eigenfunctions of localized electromagnetic modes brought about by line defects introduced into two-dimensional photonic lattices by means of the numerical simulation of their excitation process by a virtual oscillating dipole moment. In addition to quite excellent agreement with the experimental result by Lin *et al.* [Appl. Phys. Lett. **68**, 3233 (1996)], we showed that the observed localized mode has B_2 spatial symmetry. We also obtained the dispersion relation of the one-dimensional impurity band, which can be easily compared with experiments.

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Localization of radiation field in disordered photonic lattices¹ has been attracting much scientific interest.²⁻¹⁵ In addition to the novelty and the significance of the phenomenon itself, many important ideas for its technological applications such as extremely narrow-band optical filters, single-mode light-emitting diodes,² and optical waveguides with high transmittance³ fueled recent intensive investigations. The presence of photonic band gaps, or the frequency ranges where no electromagnetic mode exists, is essential for the localized modes because they become mixed with extended Bloch wave functions if their eigenfrequencies lie in the continuum of the band states. This constraint is somewhat relaxed if the polarization of the localized modes and/or the conservation of their wave vectors prevent them from being mixed with the Bloch states. The analysis of the nature of the wave functions as well as the eigenfrequencies of the localized modes is important because their optical properties such as the coupling strength to external fields and the quality factor are subject to the former.

The localized eigenmodes were found experimentally by introducing a defect to the regular dielectric structures of the photonic lattices.^{4,5} Later, several theoretical works such as impurity-band calculations based on the plane-wave expansion method,⁵⁻⁸ analyses of the transmission spectra by means of the finite-difference time-domain method,⁸⁻¹¹ and calculations of the eigenfrequencies by a real-space Green's-function method^{12,13} were reported. On the other hand, one of the present authors and his co-worker reported another method recently that is based on a numerical simulation of the excitation process of the localized modes by a virtual oscillating dipole moment located near the dielectric defect.¹⁴ This method was applied to a two-dimensional (2D) photonic lattice that had been investigated experimentally by McCall *et al.*,⁴ and excellent agreement between the experimental observation and the numerical calculation was shown for the eigenfrequency of the localized mode. In addition, the eigenfunctions with their peculiar symmetries were analyzed in detail. Memories and CPU time necessary for our method are small compared with

other methods, and accurate and efficient calculations are possible.

It is essential for our method that the eigenfrequency of the relevant localized mode is isolated since it is obtained from the resonance structure in the spectrum of the dipole radiation, and if it is close to other eigenmodes, we cannot distinguish it from them. Therefore, this method does not seem at first glance to be applicable to the problem of the impurity band that is brought about by a one-dimensional (1D) or 2D array of dielectric defects, for which the spectrum of the localized eigenmodes forms a continuum. However, we would like to show in this paper that the application of an appropriate boundary condition that matches Bloch's theorem when we solve the problem of the dipole radiation

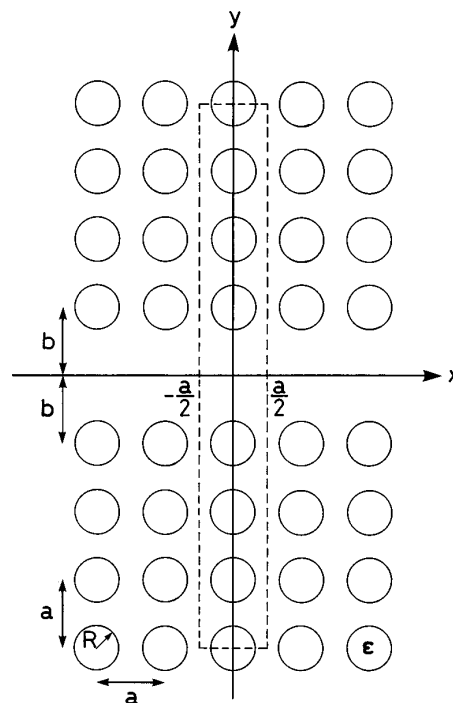


FIG. 1. The top view of the 2D square array of circular rods that was assumed for the numerical calculation (see text for details).

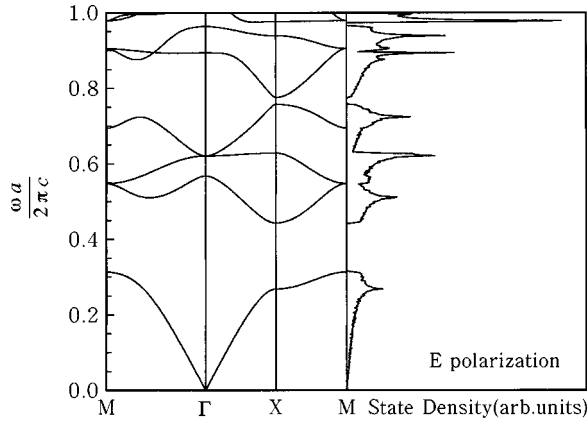


FIG. 2. The photonic band structure of the regular square lattice of the circular rods for E polarization. The ordinate is the normalized frequency. According to the experimental condition of Lin *et al.* (Ref. 15), the following values were assumed: $a=1.27$ mm, $R=0.255$ mm, $\epsilon=10.0$.

numerically leads to the distinction of a particular eigenmode with a designated wave vector. Then we will apply this method to a 1D array of defects, which will be called line defects hereafter, in a 2D square lattice that was investigated experimentally by Lin *et al.*,¹⁵ and quite excellent agreement between the experimental observation and the numerical calculation will be shown. The dispersion relation of the impurity band and the eigenfunctions will also be calculated, and the spatial symmetry of the localized mode that was found by Lin *et al.*¹⁵ will be examined.

Now, in a previous paper,¹⁴ we formulated the radiation from an oscillating dipole moment embedded in a photonic lattice that contains a dielectric defect by means of a Green's-function method developed in Ref. 16. Here, let us summarize it briefly. When we denote the eigenfunction (of the electric field) and eigenangular frequency of the localized mode by $\mathbf{E}_d(\mathbf{r})$ and ω_d , respectively, then the electric field $\mathbf{E}(\mathbf{r}, t)$ radiated from the oscillating dipole is given by

$$\mathbf{E}(\mathbf{r}, t) \approx - \frac{2\pi\omega_d \{\boldsymbol{\mu} \cdot \mathbf{E}_d^*(\mathbf{r}_0)\} \mathbf{E}_d(\mathbf{r}) \exp(-i\omega t)}{V(\omega - \omega_d + i\Gamma)}, \quad (1)$$

where $\boldsymbol{\mu}$ is the amplitude of the oscillating dipole, \mathbf{r}_0 is its position vector, ω is the angular frequency of the oscillation, Γ is the decay rate of the localized mode, and V is the volume of the lattice. When we derived Eq. (1), we assumed that ω was close to ω_d , and neglected the contribution from all other eigenmodes. On the other hand, the electromagnetic energy radiated in a unit time U is given by

$$U \approx \frac{\pi\omega_d^2 \Gamma |\boldsymbol{\mu} \cdot \mathbf{E}_d(\mathbf{r}_0)|^2}{V\{(\omega - \omega_d)^2 + \Gamma^2\}}. \quad (2)$$

Then we solve the wave equation derived from the Maxwell's equations numerically to obtain $\mathbf{E}(\mathbf{r}, t)$ and U , and we obtain ω_d from the resonance frequency of U and $\mathbf{E}_d(\mathbf{r})$ from $\mathbf{E}(\mathbf{r}, t)$.

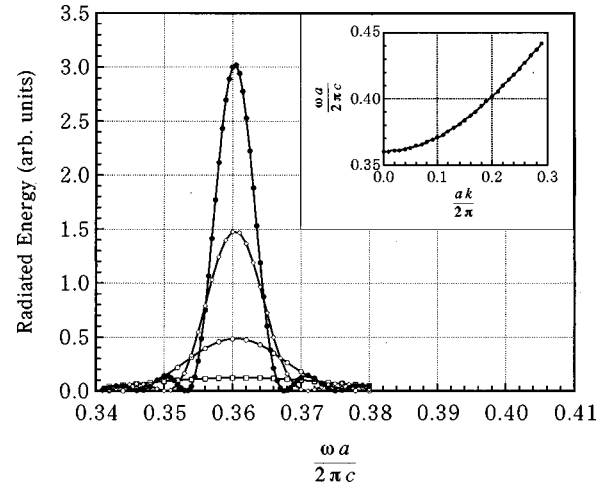


FIG. 3. The electromagnetic energy radiated by the dipole moment as a function of the oscillation frequency. \square , \circ , \diamond , and \bullet denote the accumulated electromagnetic energy after 10, 20, 35, and 50 cycles of the oscillation, respectively. The same parameters as for Fig. 2 were used. b and k were assumed to be $1.5a$ and 0 . The inset shows the dispersion relation of the 1D impurity band. Its abscissa is the normalized wave vector in the x direction.

The geometry for the present numerical calculation is shown in Fig. 1. This is the top view of a 2D square lattice composed of circular dielectric rods that was investigated by Lin *et al.*¹⁵ Here, a and R denote the lattice constant and the radius of the rods, respectively. ϵ is the dielectric constant of the rods, and that of the background (air) is assumed to be unity. The lattice is completely regular except that the distance between the centers of two layers that sandwich the x axis, $2b$, is different from a . This part of the lattice acts as the line defects. When we solve the wave equation, we assumed, according to the experimental condition of Lin *et al.*, that the electric field was parallel to the rod axis, or the z axis (E polarization). We discretized the wave equation to obtain a difference equation, and solved the latter numerically with the initial condition $E_z(\mathbf{r}, 0) = 0$. Every unit cell was divided into 40×40 parts, and one period of the oscillation was divided into 640 parts. The further decrease of the size of the spatial and temporal meshes did not give an apparent change in the eigenfrequencies of the localized modes. The area surrounded by a broken line in Fig. 1 is the supercell on which the numerical calculation was carried out. The number of the rods included in the supercell was more than 6. We imposed a boundary condition on $E_z(x, y, t)$ such that

$$E_z(x + a, y, t) = e^{ika} E_z(x, y, t), \quad (3)$$

where k is the wave vector of the localized eigenmode in the x direction. Then we could extract the contribution to the radiated electromagnetic field from this particular eigenmode with the fixed wave vector. In what follows, we will show that this simple procedure works quite well and that excellent agreement with the experimental result is obtained.

Figure 2 shows the photonic band structure of the regular (i.e., $2b=a$) square lattice of the circular rods for E polar-

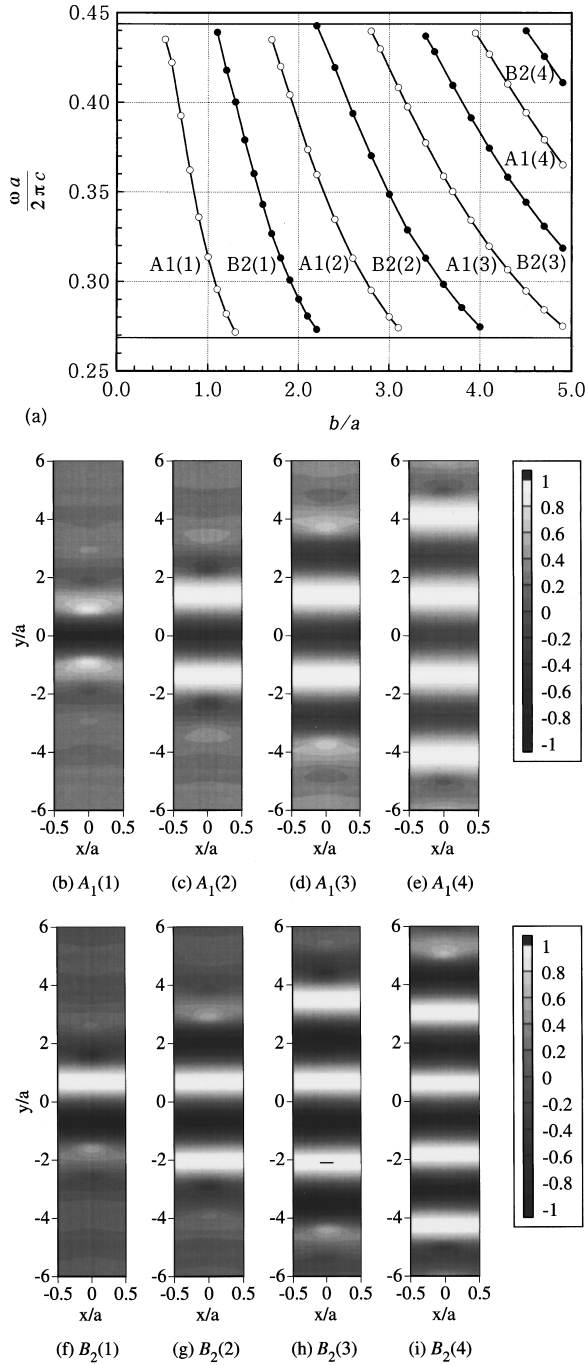


FIG. 4. (a) The eigenfrequencies at the Γ point of the 1D impurity bands as a function of the width b of the defect structure. The ordinate is the normalized frequency, and horizontal lines represent the edges of the first and second bands of the x point in the 2D Brillouin zone. The symmetry of the localized modes is also shown, where the number in parentheses is the band index that distinguishes branches with the same symmetry. (b)–(e) The distribution of the electric fields for the A_1 modes and (f)–(i) that for the B_2 modes. The maximum of each electric field is normalized to unity.

ization, which was calculated by means of the plane-wave expansion method after Plihal and Maradudin.¹⁷ 441 plane waves were used as a basis set for the band calculation, and the eigenfrequencies for 16 000 \mathbf{k} vectors in the first Brillouin zone were calculated in order to obtain the state density. The ordinate of the figure is the normalized

frequency where c denotes the light velocity in vacuum. According to the experimental condition of Lin *et al.*,¹⁵ the following values were assumed: $a = 1.27$ mm, $R = 0.255$ mm, $\epsilon = 10.0$. Figure 2 shows the presence of three band gaps. We will deal with the lowest one hereafter, since the experiment by Lin *et al.* was concerned with this band gap.

As will be shown below, the localized mode at the Γ point ($k = 0$) of the 1D impurity band found by Lin *et al.* proved to be of B_2 spatial symmetry. So, let us first examine this case, for which $b = 1.5a$. Figure 3 shows the frequency dependence of the electromagnetic energy radiated by the oscillating dipole moment located 0.2 mm apart from the origin in the y direction. Open squares, open circles, open diamonds, and closed circles denote the accumulated electromagnetic energy after 10, 20, 35, and 50 cycles of the oscillation, respectively. In this figure, we find a clear resonance at $\omega a / 2\pi c = 0.3602$, or $\omega / 2\pi = 85.03$ GHz, which is quite close to the experimental observation by Lin *et al.*,¹⁵ that is, $\omega / 2\pi = 85.5$ GHz. The discrepancy between them is less than 0.6%. On the other hand, the inset of Fig. 3 shows the calculated dispersion relation of the 1D impurity band where the abscissa represents the normalized wave vector in the x direction. In the experiments carried out by Lin *et al.*, transmission spectra of the specimen were measured with a microwave at normal incidence. Therefore, they observed the localized mode at the Γ point. If the angle of incidence is tilted, then this dispersion curve can be observed.

Next, Fig. 4(a) shows the b dependence of the eigenfrequencies of the localized modes at the Γ point where open and solid circles represent the A_1 and B_2 modes, respectively. Modes of other symmetries, i.e., A_2 and B_1 symmetries, were not found in this parameter range. In this figure, horizontal lines represent the edges of the first and second bands at the X point in the 2D Brillouin zone (see Fig. 2), between which the localized modes with $k = 0$ can exist. The number in parentheses in Fig. 4(a) is a band index in order to distinguish branches with the same symmetry. Figures 4(b)–4(e) and 4(f)–4(i) show the 2D distribution of the electric fields of the localized modes of the A_1 and B_2 symmetries, respectively. The maximum of each electric field is normalized to unity in these figures. Note that the number of the nodes of the eigenfunctions along the y axis increases with the increasing band index. Also note that the A_1 (B_2) modes are symmetric (antisymmetric) on the x axis.

In conclusion, we calculated the eigenfrequencies and eigenfunctions of the localized electromagnetic modes brought about by the line defects introduced to the 2D photonic lattices by means of the numerical simulation of their excitation process by a virtual oscillating dipole moment. In addition to quite excellent agreement between the numerical calculation and the observation by Lin *et al.*,¹⁵ we showed that the observed localized mode has the B_2 spatial symmetry. We also obtained the dispersion relation of the 1D impurity band, which can be easily compared with experiments.

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- ¹For fundamental ideas and properties of photonic lattices, see J. D. Joannopoulos, R. D. Meade, and J. N. Winn, *Photonic Crystals* (Princeton University Press, Princeton, 1995); *Photonic Band Gaps and Localization*, edited by C. M. Soukoulis (Plenum, New York, 1993); *Photonic Band Gap Materials*, edited by C. M. Soukoulis (Kluwer, Dordrecht, 1996).
- ²E. Yablonovitch, J. Opt. Soc. Am. B **10**, 283 (1993).
- ³A. Mekis, J. C. Chen, I. Kurland, S. Fan, P. R. Villeneuve, and J. D. Joannopoulos, Phys. Rev. Lett. **77**, 3787 (1996).
- ⁴S. L. McCall, P. M. Platzman, R. Dalichaouch, D. Smith, and S. Schultz, Phys. Rev. Lett. **67**, 2017 (1991).
- ⁵E. Yablonovitch, T. J. Gmitter, R. D. Meade, A. M. Rappe, K. D. Brommer, and J. D. Joannopoulos, Phys. Rev. Lett. **67**, 3380 (1991).
- ⁶D. R. Smith, R. Dalichaouch, N. Kroll, S. Schultz, S. L. McCall, and P. M. Platzman, J. Opt. Soc. Am. B **10**, 314 (1993).
- ⁷H. Benisty, J. Appl. Phys. **79**, 7483 (1996).
- ⁸P. R. Villeneuve, S. Fan, and J. D. Joannopoulos, Phys. Rev. B **54**, 7837 (1996).
- ⁹M. Sigalas, C. M. Soukoulis, E. N. Economou, C. T. Chan, and K. M. Ho, Phys. Rev. B **48**, 14 121 (1993).
- ¹⁰M. M. Sigalas, C. M. Soukoulis, C. T. Chan, and K. M. Ho, Phys. Rev. B **49**, 11 080 (1994).
- ¹¹E. Özbay, B. Temelkuran, M. Sigalas, G. Tuttle, C. M. Soukoulis, and K. M. Ho, Appl. Phys. Lett. **69**, 3797 (1996).
- ¹²A. A. Maradudin and A. R. McGurn, in *Photonic Band Gaps and Localization* (Ref. 1) p. 247.
- ¹³A. R. McGurn, Phys. Rev. B **53**, 7059 (1996).
- ¹⁴K. Sakoda and H. Shiroma, Phys. Rev. B **56**, 4830 (1997).
- ¹⁵S.-Y. Lin, V. M. Hietala, S. K. Lyo, and A. Zaslavsky, Appl. Phys. Lett. **68**, 3233 (1996).
- ¹⁶K. Sakoda and K. Ohtaka, Phys. Rev. B **54**, 5732 (1996).
- ¹⁷M. Plihal and A. A. Maradudin, Phys. Rev. B **44**, 8565 (1991).