PAPER

Size effect on light propagation modulation near band edges in one-dimensional periodic structures

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Size effect on light propagation modulation near band edges in one-dimensional periodic structures

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Periodic photonic structures can provide rich modulation in propagation of light due to well-defined band structures. Especially near band edges, light localization and the effect of near-zero refractive index have attracted wide attention. However, the practically fabricated structures can only have finite size, i.e., limited numbers of periods, leading to changes of the light propagation modulation compared with infinite structures. Here, we study the size effect on light localization and near-zero refractive-index propagation near band edges in one-dimensional periodic structures. Near edges of the band gap, as the structure's size shrinks, the broadening of the band gap and the weakening of the light localization are discovered. When the size is small, an added layer on the surface will perform large modulation in the group velocity. Near the degenerate point with Dirac-like dispersion, the zero-refractive-index effects like the zero-phase difference and near-unity transmittance retain as the size changes, while absolute group velocity fluctuates when the size shrinks.

Keywords: one-dimensional (1D) photonic crystal, finite-size effect, band gap, light localization, zero-refractive-index effect

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1. Introduction

Manipulation of light using periodic photonic structures is of fundamental interest and has attracted much research attention.[1–6] The Bragg scattering induced by the periodicity gives rise to well-defined photonic band structures, showing strong modulation on light propagation in structures. Near band edges, many intriguing effects are studied such as prohibited propagation,[3,7] light localization,[8,9] and near-zero refractive index,[10,11] etc.

Due to multiple scatterings from regions of different dielectric materials, photonic band gap appears between two band edges.[7] For frequencies among the band gap, the light is prohibited to propagate in structures. Near edges of the band gap, the photonic band shows a near-zero gradient, i.e., a near-zero group velocity, leading to the light localization.[12] For special parameters, the multiple scatterings can be counteracted, and the band gap close to be accidentally degenerate. Around the degenerate point, the band has the Dirac-like dispersion and the zero-refractive-index effect can be achieved.[13–15] These effects of light propagation modulation have been widely studied and applied in filtering,[7] confining light,[16] and enhancing light–matter interaction,[17–19] etc. It is noted that these light propagation modulation effects are usually proposed and discussed based on photonic band structures, which are strictly defined in periodic photonic structures, i.e., infinite structures. In theoretical studies, periodic boundary conditions can be adopted to match the requirement of periodicity. However, experimentally prepared structures are always finite, leading to the finite number of periods and inevitably causing some changes for the light propagation modulation in photonic structures.[20–23] A question how the light propagation modulation properties vary when the structure changes from the infinite to the finite arises. The study on the size effect is to depict the change of optical properties when the finite structure's size varies. For one-dimensional (1D) structures, there have been numerous studies on the optical properties when the size of the structures varies. The number of the hole rings[24] and the core size[25,26] were changed to optimize the properties of the photonic crystal fibers, and two 1D finite structures contacted together show the robustness of the interface states when the size varies.[27] However, to date the size effect of the modulation properties of photonic structures has still not been fully discussed.

In this work, we study the size effect of light propagation near the band edges in 1D periodic structures. The broadening of the effective band gap is observed when a structure becomes small. Then the group velocity is introduced to discuss the light localization modulation near edges of the band gap. As the structure's size shrinks, the group velocity increases, corresponding to the weakening of light localization. When the size is small, a layer added on the surface will perform a relatively large modulation in the group velocity. For the degenerate point with Dirac-like dispersion, the zero-refractive-index effects like zero phase difference and near-unity transmittance

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keep unchanged as the structure's size varies, while the corresponding group velocity fluctuates when the size shrinks.

2. Results and discussion

The size effect is discussed in the 1D periodic structure, as shown in Fig. 1(a). The unit cell consists of two different layers. For layer A, the refractive index n_A is 1.45 and the thickness d_A is 289.7 nm. For layer B, the refractive index n_B is 2.1 and the thickness d_B is 200 nm. By using the transfer matrix method,[28] the equation of the band structure is derived as

$$\cos(kd) = \cos\left(\frac{\omega}{c}n_\mathrm{A}d_\mathrm{A}\right)\cos\left(\frac{\omega}{c}n_\mathrm{B}d_\mathrm{B}\right) - \frac{n_\mathrm{A}^2+n_\mathrm{B}^2}{2n_\mathrm{A}n_\mathrm{B}}\sin\left(\frac{\omega}{c}n_\mathrm{A}d_\mathrm{A}\right)\sin\left(\frac{\omega}{c}n_\mathrm{B}d_\mathrm{B}\right), \quad (1)$$

where k, d, ω, and c refer to the Bloch wave vector, the period of the structure, the angular frequency, and the speed of light in vacuum, respectively. It is noted that optical paths of two layers are set to be equal to each other, i.e., $n_\mathrm{A}d_\mathrm{A} = n_\mathrm{B}d_\mathrm{B}$, hence the band gap and degenerate point with Dirac-like dispersion can be discussed in the same structure. As is shown in Fig. 1(b), a band gap is observed at the boundary of the first Brillouin zone, and a degenerate point (marked by red dot) with Dirac-like dispersion is observed at the center of the Brillouin zone.

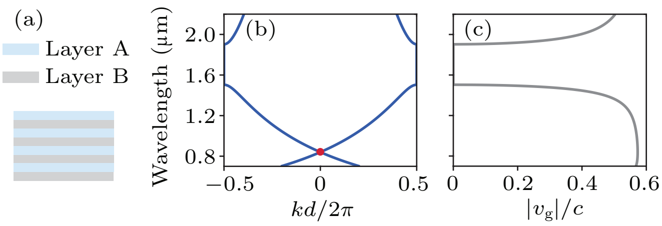

Fig. 1. (a) Schematic of the 1D periodic structures. (b) The photonic band structure. The red point marks a degenerate point. (c) The derived absolute group velocity.

Figure 1(c) shows the absolute value of the group velocity $|v_\mathrm{g}|$, from which the propagation features like localization can be analyzed. In the band gap, the light propagation is prohibited, hence the $|v_\mathrm{g}|$ is ill-defined. When close to the band edges from the outside of the band gap, we can see that the $|v_\mathrm{g}|$ decreases rapidly and becomes zero at band edges, indicating that the light propagates slowly near band edges and gets strongly localized at band edges. Diversely, near the degenerate point with Dirac-like dispersion, $|v_\mathrm{g}|$ remains at a non-zero value and keeps nearly-unchanged. This can be understood from the linear dispersion relation, which would also lead to the zero-refractive-index effect.[10,11,13–15] Up to now, all these properties are discussed based on well-defined band structures of infinite structures. To discuss how light propagation modulation properties change when the structures become finite, the finite-size simulations are further performed.

The finite-difference time-domain method is employed to study light propagation in structures with finite size in both frequency and time domains. The size of the 1D structures is characterized by the number of layers (N). For the frequency domain, the transmittance spectra and the intensity distributions of electric field can be calculated. For the time domain, the group velocity can be obtained as follows:[29,30] A light pulse with 2-nm full width at half maximum is simulated to pass through the finite structure and the vacuum of the same distance respectively. Then the time delay can be extracted by comparing the time difference of these two pulses, from which the group velocity of light propagating in the structures can be obtained.

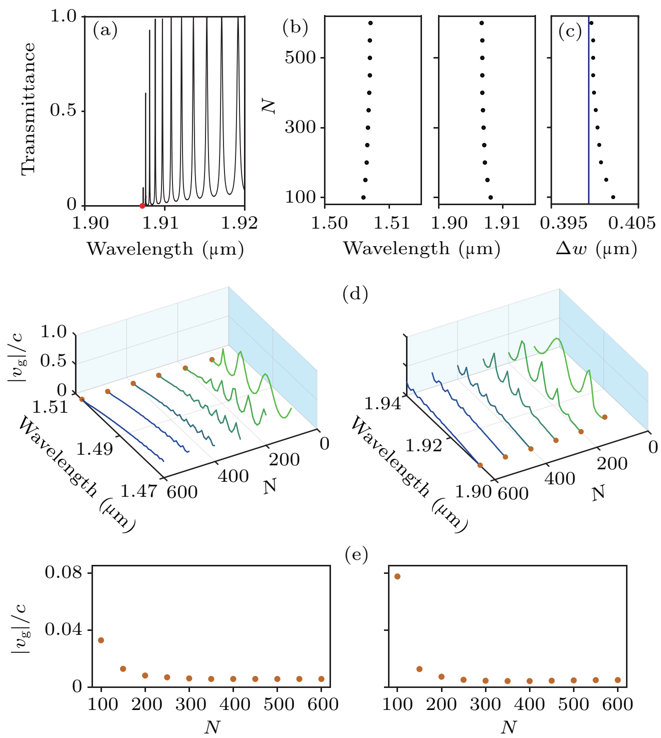

Fig. 2. Transmittance spectrum of the structure with 600 layers. The red point marks the effective band edge. (b) The band edges of different N. (c) The width of the band gap with different N. Δw denotes the bandgap width, and the blue line represents the width of band gap of the infinite photonic structure. (d) Group velocity near edges of the band gap. The orange dots represent the group velocity at the band edges. (e) Group velocity at the band edge of the structures. The left and the right panels show the group velocity at the short-wavelength and the long-wavelength edges, respectively. N denotes the number of layers.

Figure 2(a) shows the transmittance spectrum near the long-wavelength edge when N is 600. The transmittance exhibits large fluctuations. In the band gap, the transmittance decreases to be zero due to the prohibited propagation. As indicated by the red point, the effective band edge is chosen when the transmittance is 0.01. Figure 2(b) plots the evolution of effective band edges with changing N. The slight narrowing of the band gap is observed with increasing N. To get a deeper insight into the change of the band gap, the widths of the band gap (Δw) are shown in Fig. 2(c). As N increases, the width of the band gap approaches the calculation by the transfer matrix. This decreasing difference between the two widths of the band gap can represent the smaller difference between the finite structures and the infinite ones. Then, Fig. 2(d) presents the group velocity near band edges of finite structures with different N. For each N, group velocity decreases when the wavelength approaches close to the band gap, while the group velocity shows larger fluctuations for structures with smaller N. Furthermore, Fig. 2(e) plots the group velocity at defined effective band edges. It could be seen that the group velocity decreases as the structure's size increases and approaches to a nearly unchanged minimum value. It should be mentioned that the non-zero minimum is due to the non-zero frequency width of the simulated pulses. As we can see, the calculated group velocity is far less than the light velocity in vacuum, showing the light localization modulation at band edges. The light is more localized at band edges for structures with more layers.

To gain a deeper insight into the light localization at band edges, we calculated the intensity distributions of the electric field at effective band edges in structures of different N considering a monochromatic incident light, as shown in Figs. 3(a) and 3(b). The left, middle and right panels correspond to the structures whose N are 100, 200, and 600. For comparison, the intensity distribution are all exhibited within 15 μm from the incident surface, while the intensity distribution of entire structures are shown in the inset of each panel. For the largest structures with 600 layers, the intensity decays exponentially from the incident boundary, showing obvious localization behavior. In contrast, for structures with smaller N, the intensity decay more slowly, indicating weaker localization modulation. The results are in accordance with the group velocity discussions in Fig. 2(d).

When structures become finite, the backward-propagating waves by the other boundary would also influence the total light propagation modulation. The boundary effect was studied by considering an added layer on incidence surface. As is illustrated in the inset of Fig. 3(c), the added layer is firstly a layer with refractive index n_B and the thickness varying from 0 to d_B, then another layer with the refractive index n_A and the thickness varying from 0 to d_A. Figure 3(c) shows that the group velocities at the short-wavelength (black dots) and the long-wavelength (red dots) band edges. It could be seen that the group velocity in the structure of a smaller size exhibits a larger variation with the varying added layer. This boundary effect is an evident difference between the finite and the infinite structures. The added layer could be considered as an additional degree of freedom to modulate the light propagation for structures of a small size.

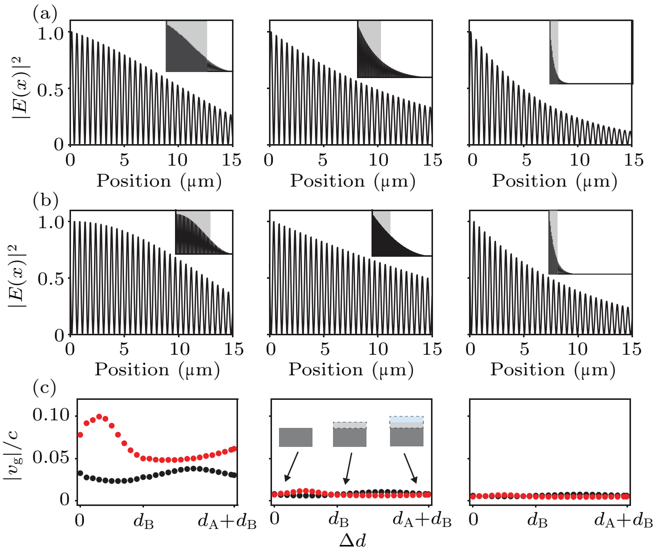

Fig. 3. Intensity distributions of the electric field at (a) the short-wavelength and (b) the long-wavelength edges of the band gap. The insets show the intensity distributions inside the entire structures, and the main figures are the zoom-in views of the shadow areas of the insets. (c) Group velocity at the short-wavelength (black dots) and the long-wavelength (red dots) band edges with the change Δd on the surface. The inset shows the schematics when Δd is 0, d_B and $d_A + d_B$. N of the structures in the left, the middle and the right panels are 100, 200 and 600, respectively.

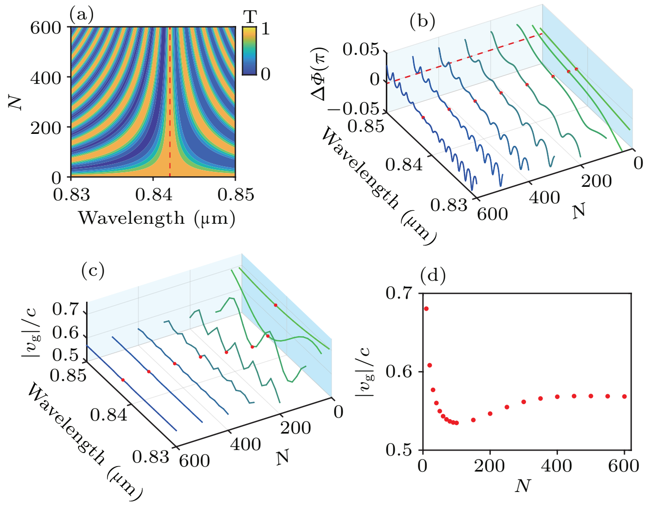

Fig. 4. (a) Transmittance spectra of structures of different N. (b) Phase differences $\Delta\Phi$ between the top and the bottom surfaces in one unit cell with different N. The red dots and the dashed line indicate the zero phase difference at 0.842 μm. (c) Group velocity of the structures with different N. The red dots show the group velocity at 0.842 μm. (d) Group velocity at the degenerate point of the structures with different N.

Further, the size effect around the degenerate point with Dirac-like dispersion is discussed. For the ideal zero-refractive-index material, the near-unity transmittance and zero phase difference are enabled by the zero effective refractive index.[10,11] Figure 4(a) shows the transmittance spectra of varying N. It can be seen that as the near-unity transmittance (red dashed line) is maintained, and the wavelength is in accordance with that of the degenerate point in Fig. 1(b). Then we calculated the phase difference between two boundaries of a unit cell, as is shown in Fig. 4(b). The zero phase difference is kept to be unchanged despite the varying N. For the degenerate point with Dirac-like dispersion, these zero-refractive-index effects shows little difference between the finite and the infinite structures. In addition, the group velocity are also simulated, as is shown in Fig. 4(c). Similar to the results near the band gaps, the group velocity exhibits obvious fluctuations when N is small. The group velocity at the degenerate point is plotted in Fig. 4(d). With increasing N, the group velocity approaches to a non-zero value of $0.57c$. This value agrees well with the calculated group velocity of the infinite structures in Fig. 1(c).

3. Conclusion

In summary, the size effect of light propagation modulation in 1D periodic structures is studied. The light propagation modulation properties vary when the structures become finite. As the structure's size shrinks, near band edges of the band gap, the light localization weakens, and the boundaries of the finite structure perform an obvious modulation on the total group velocity in structures. For the degenerate point with Dirac-like dispersion, the zero-refractive-index effect like near-unity transmittance and zero phase difference keep unchanged in finite structures with the varying size, while the group velocity suffers fluctuations when size is small. The result reveals that the light propagation modulation properties, especially the group velocity modulation in periodic structures, get changed when the periodic structure's practical size becomes finite. It also reminds that the finite size effect should be considered when the periodic structures with the actually finite size are practically applied.

Acknowledgements

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References

[1] John D J, Johnson S G, Winn J N and Meade R D 2008 *Photonic crystals: Molding the flow of light* 2nd edn. (Princeton: Princeton University Press)
[2] Lova P, Manfredi G and Comoretto D 2018 *Adv. Opt. Mater.* **6** 1800730
[3] Notomi M 2010 *Rep. Prog. Phys.* **73** 096501
[4] Erdiven U, Tetik E and Karadag F 2018 *Chin. Phys. B* **27** 044204
[5] Ye W M, Luo Z, Yuan X D and Zeng C 2010 *Chin. Phys. B* **19** 054215
[6] Tang Z X, Fan D Y, Wen S C, Ye Y X and Zhao C J 2007 *Chin. Opt. Lett.* **5** S211
[7] Maigyte L and Staliunas K 2015 *Appl. Phys. Rev.* **2** 011102
[8] John S 1987 *Phys. Rev. Lett.* **58** 2486
[9] Haberko J, Froufe-Pérez L S and Scheffold F 2020 *Nat. Commun.* **11** 4867
[10] Liberal I and Engheta N 2017 *Nat. Photon.* **11** 149
[11] Vulis D I, Reshef O, Camayd-Muñoz P and Mazur E 2018 *Rep. Prog. Phys.* **82** 012001
[12] Baba T 2008 *Nat. Photon.* **2** 465
[13] Huang X Q, Lai Y, Hang Z H, Zheng H H and Chan C T 2011 *Nat. Mater.* **10** 582
[14] Li Y, Kita S, Muñoz P, Reshef O, Vulis D I, Yin M, Lončar M and Mazur E 2015 *Nat. Photon.* **9** 738
[15] Minkov M, Williamson I A D, Xiao M and Fan S H 2018 *Phys. Rev. Lett.* **121** 263901
[16] Russell P 2003 *Science* **299** 358
[17] Johnson C M, Reece P J and Conibeer G J 2011 *Opt. Lett.* **36** 3990
[18] Zhang W, Anaya M, Lozano G, Calvo M E, Johnston M B, Míguez H and Snaith H J 2015 *Nano. Lett.* **15** 1698
[19] Mattiucci N, Bloemer M J and D'Aguanno G 2014 *Opt. Express* **22** 6381
[20] Bertone J F, Jiang P, Hwang K S, Mittleman D M and Colvin V L 1999 *Phys. Rev. Lett.* **83** 300
[21] Galisteo-López J F, Palacios-Lidón E Castillo-Martínez E and López C 2003 *Phys. Rev. B* **68** 115109
[22] Liang Y, Peng C, Sakai K, Iwahashi S and Noda S 2012 *Opt. Express* **20** 15945
[23] Miranda-Muñoz J M, Esteso V, Jiménez-Solano A, Lozano G and Míguez H 2020 *Adv. Opt. Mater.* **8** 1901196
[24] Désévédavy F, Renversez G, Troles J, Houizot P, Brilland L Vasilief I, Coulombier Q, Traynor N, Smektala F and Adam J L 2010 *Opt. Mater.* **32** 1532
[25] Knight J C, Arriaga J, Birks T A, Ortigosa-Blanch A, Wadsworth W J and Russell P S J 2000 *IEEE Photon. Technol. Lett.* **12** 807
[26] Poletti F, Petrovich M and Richardson D J 2013 *Nanophotonics* **2** 315
[27] Kalozoumis P A, Theocharis G, Achilleos V, Félix S, Richoux O and Pagneux V 2018 *Phys. Rev. A* **98** 023838
[28] Yeh P, Yariv A and Hong C S 1977 *J. Opt. Soc. Am.* **67** 423
[29] Imhof A, Vos W L, Sprik R and Lagendijk A 1999 *Phys. Rev. Lett.* **83** 2942
[30] Dal Negro L, Oton C J, Gaburro Z, Pavesi L, Johnson P, Lagendijk A, Righini R, Colocci M and Wiersma D S 2003 *Phys. Rev. Lett.* **90** 055501