Uncoupling Spectral Region in Two-Dimensional Square Lattice Photonic Crystals

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Recently photonic crystals draw the attentions of researchers because of their potential for various applications [1–3]. Originally, they opened the possibility of manipulating propagation processes as well as electromagnetic wave emission. Photonic crystals show rich anomalous dispersion characteristics such as negative dispersion and super-prism phenomena [4–9]. It is well known that inside a photonic bandgap, no photon state is allowed and all the incident photons should be reflected [10–12]. Here, we report that one can achieve total reflection even without the help of the photonic bandgap. This idea relates to the heavy anomalous dispersion in photonic crystals. In fact, the same phenomenon for the two-dimensional case was already observed in other papers but we used different approaches [13,14]. We will call this spectral region 'uncoupling spectral region' inside which light cannot couple to photonic crystals from air. Here, we investigated this effect in two-dimensional (2D) square photonic crystals for various ranges of holes and rods by theoretical calculation. It is interesting that although a complete bandgap does not exist, a complete total bandgap (common bandgap in both TE and TM modes with the help of the uncoupling spectral region) can be observed from 2D square lattices.

To start, we choose a 2D square lattice photonic crystal of holes or rods with lattice constant $a$. Consider photons that are incident on a surface of a photonic crystal from the air. For a 2D square lattice air hole structure, a typical band diagram for transverse electric (TE) modes is shown in Fig. 1(a). 2D plane wave expansion methods are used for this calculation (20 plane waves are used in each $x$ and $y$ direction). Here the dielectric constant is 10.5 and the hole radius is 0.4$a$. In order to understand the refraction phenomenon at the air-photonic crystal interface, it is useful to draw an eigen-frequency contour in the 2D momentum space, as shown in Fig. 1(b) ($a/\lambda = 0.26$ in this case). The open circles represent the dispersion surface in the air, which is based on the isotropic dispersion relation of the air, $\omega = c(k_x^2 + k_y^2)^{1/2}$. The four arcs (closed-squares) formed at the four corners are the dispersion surfaces of the photonic crystal. Note that these eigen-frequency contours are discontinuous and extremely anisotropic. Also the effective refractive indices (the distance from the origin) of the four regions are larger than that of the air. In fact, these points in Fig. 1(b) show all the possible propagation states inside the photonic crystal at a frequency of $a/\lambda = 0.26$.

Now suppose that light is incident on the 2D square photonic crystal surface with an angle $\theta$ with respect to the (01) direction shown in the inset of Fig. 1(b). In $k$-space, this situation can be represented by drawing an arrow pointing at the same angle $\theta$ with respect to the $k_x$-axis as shown in Fig. 1(b). To understand light propagation through the interface of two materials, one needs to apply the conservation condition of the tangential component of the $k$ vector. The dotted vertical line $a$ in Fig. 1(b) graphically represents all the $k$-space points satisfying the condition of $k_x$ conservation. The light incident on the photonic crystal surface can propagate only if it can find the corresponding $k_x$ on the eigen-frequency contour of
the photonic crystal. For an example of $a/\lambda = 0.26$, the light from the air cannot find any allowed photon state inside the photonic crystal since the eigen-frequency contour of the photonic crystal does not have any cross point with the vertical momentum conservation line. Consequently, this spectral region near this frequency disallows the light coupling from air into the photonic crystal. Note in Fig. 1(a) that $a/\lambda = 0.26$ lies outside of the photonic bandgap. We named this forbidden spectral region 'uncoupling spectral region'. The uncoupling effect is noticeable until $a/\lambda$ becomes 0.221, as indicated in Fig. 1(a). When $a/\lambda$ equals 0.221, the incident angle from the air should be $90^\circ$ to find a corresponding state inside the photonic crystal. As the frequency becomes smaller than 0.221, more propagation states become available. It is worth pointing out that this phenomenon is different from the total internal reflection. The effective refractive index inside the uncoupling region is always larger than that of air.

To understand the general situations of different incident materials and surfaces of the photonic crystal, consider the incident light generated at a point A in a dielectric material, which is connected to the photonic crystal as indicated in the inset of Fig. 2(a). In this case, the radius of the equal-frequency circle in the dielectric material increases by a factor of $n$ that is the refractive index of the dielectric material as shown in Fig. 2(a). So, the light generated at the point A can find allowed photon states inside the photonic crystal. For comparison, if the photon is generated in the air (point B) as shown in the inset of Fig. 2(a), this photon cannot propagate through the photonic crystal because the phase matching condition at an interface.

FIG. 1. (a) The band diagram of a 2D square hole structure for TE polarization. The incident light cannot be coupled to the photonic crystal in the frequency region below the original bandgap. The uncoupling region extends down to $a/\lambda = 0.221$. (b) Dispersion surfaces of air and the photonic crystal (depicted in the inset) for $a/\lambda = 0.26$.

FIG. 2. (a) Eigen-frequency contour for light sources located inside the dielectric material. The point A is not in a photonic crystal but in a dielectric material (b) The momentum conservation line should be drawn perpendicular to the surface of the air/photonic crystal interface.
between air and the material cannot be satisfied. In fact, the momentum conservation line in 2D k-space should be drawn perpendicular to the plane of incidence. If light is incident on a different surface with an angle $\alpha$ as depicted in the inset of Fig. 2(b), the direction of momentum conservation line in k-space is changed as the line $b$ shown in Fig. 2(b). Note that the uncoupling region disappears in this case.

In fact, one can find an uncoupling region for transverse magnetic (TM) modes as well. For a 2D square lattice air hole structure in which a dielectric constant is 10.5 and the hole radius is 0.4$a$, a band diagram and eigen-frequency contour ($a/\lambda = 0.225$) for TM modes is shown in Fig. 3. Fig. 3(b) shows the existence of a common uncoupling region for both the TM and TE modes. Let’s define the total bandgap as an addition of this uncoupling region and the true bandgap. From a square lattice of air holes with radius $r = 0.4a$, one can even find the common total bandgap for the TE and TM modes in common. We would like to name this region the complete total bandgap. The gap-midgap ratio of this complete total bandgap of the square lattice photonic crystal represents the width of the bandgap. Fig. 4(a) shows the gap-midgap ratio of a complete total bandgap for a square lattice of dielectric constant 13. The gap-midgap ratio remains large when the radius of air holes varies from 0.3$a$ to 0.4$a$. The size of the complete total bandgap increases with the dielectric constant as shown in Fig. 4(b). This result is obtained when $r = 0.35a$. Compare the result at dielectric constant 13 with the gap-midgap ratio when $r = 0.35a$ in Fig. 4(a). When the dielectric constant $\varepsilon$ becomes smaller than 7, no complete total bandgap is found. The index difference between air and the photonic crystal is an important factor for the formation of the uncoupling region.

![Fig. 3](image_url) (a) The band diagram of a 2D square hole structure for TM polarization. (b) Dispersion surface of air, TE modes and TM modes at $a/\lambda = 0.225$.

![Fig. 4](image_url) (a) Gap-midgap ratios of a complete total bandgap for a 2D square lattice ($\varepsilon=13$). Around $r = 0.35a$, the gap-midgap ratio becomes maximum. (b) The variation of the complete total bandgap ($r = 0.35a$) with dielectric constant. The region between the upper band edge (closed squares) and the lower band edge (opened squares) is the complete total bandgap.
FIG. 5. The projected complete total bandgap as a function of a $k_z$-component for a square holes lattice. Between the open spots and closed spots is the bandgap.

By now, we reported uncoupling phenomenon in 2D where an incident light from air on only $z$-$y$ 2D plane is reflected without the help of the photonic bandgap. In order to expand this concept to three-dimensions, we examine the variation of the complete total bandgap with non-zero $k_z$ component as shown in Fig. 5. The condition is indicated in the inset of Fig. 5. The region between open squares and closed squares is the complete total bandgap. The radius of air holes is $0.34a$ and dielectric constant is 13. Three-dimensional (3D) plane wave expansion method is used for this calculation with 16, 16 and 80 plane waves in $x$, $y$ and $z$ directions respectively. The region below the light line ($\omega = ck_z$) can be neglected because the light incident from air has imaginary $k_x$, $k_y$ components. In the region above the light line, the complete total bandgap tends to become smaller with $k_z$. We can even find an omni-directional region where the incident light from all 3D directions is totally reflected [15-17]. In the shaded region shown in Fig 5, the photonic crystal acts as an omni-directional mirror for all polarizations.

In summary, we have introduced the uncoupling phenomenon in 2D square photonic crystals and have examined characteristics of the uncoupling spectral region. Under the condition that the momentum conservation line is parallel to $X$-$M$ (or $\Gamma$-$X$), most square lattice photonic crystals have an uncoupling region. We found that the size of the complete total bandgap (common bandgap in both TE and TM modes) of a square lattice can be made as large as that of the complete bandgap of triangular lattice. We also found the omni-directional frequency region of the complete total bandgap in a square hole lattice photonic crystal. This uncoupling effect is expected to find various interesting applications.

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