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DESIGN AND MODELING FOR ENHANCEMENT OF LIGHT EXTRACTION IN LIGHT-EMITTING DIODES WITH ARCHIMEDEAN LATTICE PHOTONIC CRYSTALS

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Abstract—Light extraction efficiency of light-emitting diodes (LEDs) based on various photonic crystal (PhC) structures is investigated in this study. By using the plane wave method and the finite element method, the influence of several factors on the enhancement of light extraction is discussed, including lattice type, the density of states from a photonic band diagram, the ratio of cylinder radius and lattice constant, and the thickness of a PHC pattern. Some rules are given for the practical implementation of an optimized PhC-based LED with higher light extraction efficiency. In the simulation results, the maximum enhancement of the extraction efficiency could be by a factor of approximately 2.8 for the optimized Archimedean tiling pattern in the LED device emitting at the center wavelength of 530 nm. However, with the use of optimized PhC structures, the square and triangular lattices reveal enhancements of ~ 1.7 and ~ 1.5, respectively. The extraction efficiency of the Archimedean PhC LED is much greater than that of the regular lattice PhC LED.

1. INTRODUCTION

Photonic crystals (PhCs) allow one to enhance, attenuate, or suppress spontaneous emission properties of materials placed inside them [1]. They can control the spatial distribution of radiation power and redistribute the spectrum of the emitted light into useful forms. The ability to manipulate light emission has potentials on many optoelectronics devices [2].

Light-emitting diodes (LEDs), which spontaneously emit radiation from a *p*-*n* junction, have attracted much interest for a wide range of applications in solid-state lighting, displays, optical communications, and optical interconnects in computers. The light outcoupling efficiency of LEDs has important consequences on such applications. Unfortunately, most of the light emitted from conventional surface-emitting LEDs is mainly limited by the total internal reflection within the high dielectric material, leading to a poor external efficiency. The need for the improvement of light extraction efficiency is exceptionally significant. Much effort has been exerted to overcome this limit, including surface texturing, the use of microlenses, reshaping the light escape cone, distributed feedback structures, and the diffraction by a two-dimensional (2D) PhC [3–6]. In particular, high light-extraction efficiency is expected for the integration of 2D PhCs, which allows the control of photonic behavior in a predictable manner.

PhCs have a periodic dielectric modulation with a spatial scale on the order of the optical wavelength. Design and optimization of the PhCs are not simple due to the multi-parameter problem of a patterned texture. There are many factors related to the combinations of intermixing materials, lattice symmetry, lattice constant, filling factor, shape of the scattering object, and thickness of a PhC layer. It is not easy to say which one provides the most efficient PhC structure in the improvement of light extraction efficiency in LEDs. There are two main options to improve light extraction by means of PhCs: the first one is the use of the photonic band-gaps (PBGs) to enhance emission in useful directions and to inhibit it in others; the other is to redirect the emission from guided modes into radiative modes [7]. Nevertheless, the first effect generally leads to nonradiative losses and the requirement of a sufficiently large refractive index contrast to open a full band-gap [8]. Hence, the second option is considered here for the advantage of being compatible with present material processes and amenable to treatment in real components.

The introduction of periodic patterning within the LED device causes the dispersion curves of Bloch modes to become folded at the Brillouin zone boundary. Thus, some of the wave-guided modes (trapped modes lying below the light line) will be shifted to the diffracted modes lying above the light line and escape from the device [2]. Photonic quasi-crystals (PhQs) are similar to PhCs but rely on a quasi-crystal arrangement of scattering objects [5, 9–11]. PhQs possess high symmetry orders not achievable in nature and offer many desirable features, such as isotropic PBGs, operation in low refractive index materials, diffraction not arising from the nearest neighbor dielectric rod interactions, and flat dispersion bands. However, it is difficult to numerically establish the dispersion properties of most PhQs. Archimedean lattices are a category of PhQs, consisting of regular convex polygons which are not necessarily identical and can fill the whole plane without gaps [11]. There are 11 Archimedean tilings, including the familiar traditional Bravais lattices: square, triangular, and honeycomb structures. The benefits of Archimedean lattices are a higher order of local rotational symmetry than the regular lattices and the strict periodicity which allows the calculation of the dispersion relations by numerical methods. Besides, the isotropic behaviors can be transposed to light-diffracting PhQs, and the lattice constants can reach the wavelength of visible light.

In this work, we present a different approach to the optimization of light extraction efficiency in the LEDs through PhCs (PhQs). A kind of simple 2D PhC structure constructed with a small portion of PhQs is proposed for the quasi omnidirectionality of light extraction. In addition, this numerical study is targeted to examine the light extraction efficiency of the LEDs based on different kinds of basic PhC structures and the proposed PhQ one, and to find the most effective design under optimized parameters for further discussion. Taking a typical organic LED device as an illustration, the introduction of PhCs (PhQs) to the improvement of extraction efficiency is discussed in detail. The relevance between the predictions of the plane wave method (PWM) [1] and the consequences of the three dimensional finite element method (3D FEM) calculation is demonstrated for highly efficient light-extracting structures. The simulation results reveal that the PhQ-based LEDs show higher light output than the traditional PhC-based ones.

2. SIMULATION MODEL AND METHOD

The theoretical study of photonic structures is based on the three geometrical configurations shown in Fig. 1, i.e., square, triangular, and Archimedean $(4, 8^2)$ arrays of circular cylinders. The notation to categorize the Archimedean lattices is a set of shape and number of polygons $(n_1^{a_1}, n_2^{a_2}, n_3^{a_3}, \ldots)$, denoting a tiling of a vertex type in the way that n_1-gon, n_2-gon, and n_3-gon, ..., meet clockwise on each vertex, and the superscript a_i refers to the number of these polygons adjacent to each other [12]. The symbol $(4, 8^2)$ means a tiling in which a square and two octangles gather edge-to-edge around a vertex. The $(4, 8^2)$ lattice has been also called the "bathroom tile" lattice, and its photonic structure is obtained by the placement of dielectric cylinders at the vertices. Four parameters are involved in the simulation: lattice constant a, emitting center wavelength λ, thickness d of a pattern array, and ratio ($f = r/a$) of radius and lattice constant, where r is the radius of the circular cylinders.

As can be seen from Fig. 1(c), such a periodic structure can be also considered as clusters of 4 atoms organized in a square Bravais lattice. This indicates that Wigner cells can be defined and all the theoretical and numerical methods can be applied to model the multiple wave scattering. Photonic band structures can be calculated by defining periodically supercells. The primitive cell is formed through two primitive translation vectors $\mathbf{a}_1 = (1 + 1/\sqrt{2})a(1, 1)$ and $\mathbf{a}_2 = (1 + 1/\sqrt{2})a(-1, 1)$. The positions of the cylinders in the unit supercell with respect to the coordinate origin are $\mathbf{u}_1$, $\mathbf{u}_2$, $\mathbf{u}_3$ and $\mathbf{u}_4$ with $\mathbf{u}_1 = a(1/2, (1/2 + 1/\sqrt{2}))$, $\mathbf{u}_2 = a(1/2, -(1/2 + 1/\sqrt{2}))$, $\mathbf{u}_3 = a(-1/2, -(1/2 + 1/\sqrt{2}))$, and $\mathbf{u}_4 = a(-1/2, (1/2 + 1/\sqrt{2}))$, respectively. For any integers $l_{1,2}$, $\mathbf{R} = l_1\mathbf{a}_1 + l_2\mathbf{a}_2$ defines the Bravais lattice with the periodic dielectric constants $\varepsilon(\mathbf{r} + \mathbf{R}) = \varepsilon(\mathbf{r})$, where $\mathbf{r}$ is the position vector. A standard PWM can be used to calculate the band diagrams.

There are several positions in which a PhC (PhQ) can be inserted in to an LED device [4]. For practical applications, the introduction of a PhC (PhQ) in the anode layer should be the most effective, as it does not lead to a modification in the electronic properties of the device. Besides, the light emitted from the LED device can be classified into the following modes: the radiation mode, the surface plasmon mode, the waveguide mode, and the substrate mode [4, 13]. From the theoretical

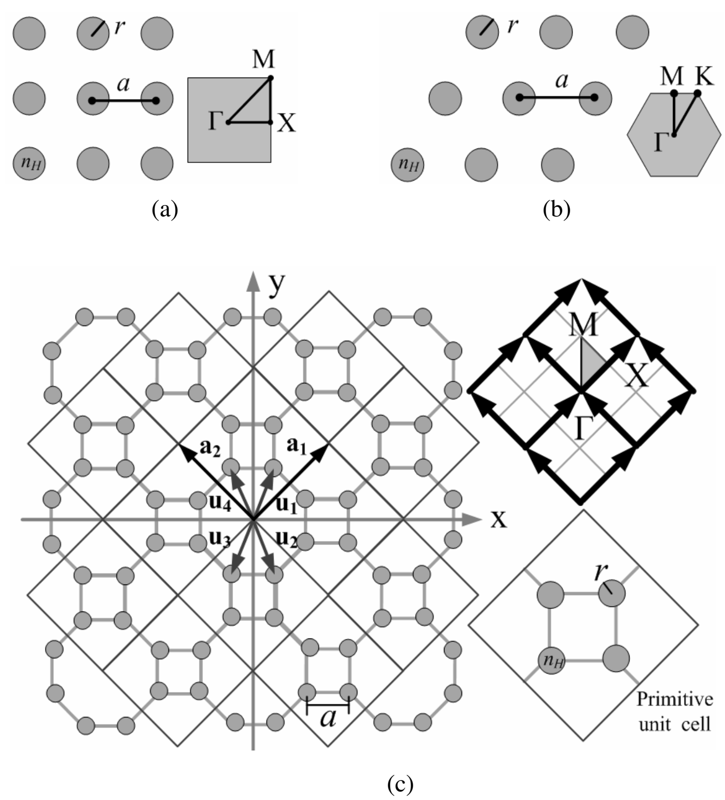

Figure 1. Various PhC/PhQ lattice tiling schemes and their corresponding unit cells in reciprocal space: (a) square lattice; (b) triangular lattice; (c) $(4, 8^2)$ Archimedean lattice. These photonic structures with lattice constant a are composed of cylinders with a refractive index of $n_H = 1.95$ and a radius of $r = fa$. The substrate refractive index is $n_L = 1.48$. The primitive cell in (c) including four cylinders is defined by two primitive translation vectors $\mathbf{a}_1$ and $\mathbf{a}_2$. Four cylinders surrounding the coordinate origin are at positions $\mathbf{u}_1$, $\mathbf{u}_2$, $\mathbf{u}_3$, and $\mathbf{u}_4$, respectively.

analysis, the latter two modes have the largest portion of the emitted light, which is confined inside the device [4]. In order to effectively extract the light, the PhC (PhQ) formed between the substrate and anode layers could realize the enhancement of luminance efficiency. At this interface, the PhC (PhQ) structure can have a strong influence on the extraction of the light trapped in the waveguide mode and the substrate mode [14].

In order to study the emission characteristics, the 3D FEM via the COMSOL™ simulation software is employed for the numerical analysis of the LED device. This method can be used to describe optical properties observable in complex structures. A schematic diagram of the general organic LED structure [15–17] shown in Fig. 2 is adopted for simulation. The trial for improving the light extraction efficiency is aimed at the incorporation of the 2D PhC (PhQ) layer inside the conventional organic LED, consisting of a glass substrate, a 2D SiO_2 ($n_L = 1.48$)/SiN_x ($n_H = 1.95$) PhC (PhQ) layer, an indium-tin-oxide (ITO) anode ($n = 1.8, 150\,\text{nm}$ thick), an organic emitting layer ($n = 1.75, 145\,\text{nm}$ thick), and a metal cathode. The light-emitting excitons placed in the LED are represented by dipoles, which are located at the center of the active layer and are aligned along the horizontal (x and y) and the vertical (z) directions. Lagrange-quadratic elements are chosen as the basis elements. The discrete model is based on a mesh limit with $\Delta x, \Delta y, \Delta z \leq \lambda/(10n)$, where λ is the vacuum wavelength. For the simplification of calculation and modeling, absorbing boundary conditions are used, and the optical absorption in each layer is neglected. Due to the limitation of computer memory capacity, the thickness of the glass substrate is set to be $5\lambda_g$, and the lateral region size for the FEM computation is simulated with a

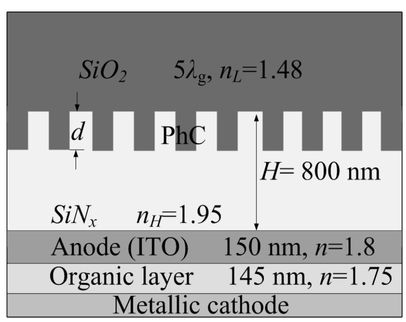

Figure 2. Schematic cross-sectional view of the organic LED employing a 2D SiO_2/SiN_x PhC(PhQ) slab. The specified refractive indices are relative to the emitting wavelength of $\lambda_g = 530\,\text{nm}$.

5×5 lattice array. The results of band diagram calculations, especially the density of states (DOS) in the radiation mode, are related to the transmission properties calculated with the 3D FEM.

3. OPTICAL CHARACTERISTICS AND RULES OF DESIGN

The introduction of various periodic structures is to create a frequency range for which no guided modes can exist. In this frequency range, all the emitted light will couple to free space modes. A calculated photonic band diagram in transverse electric (TE) and transverse magnetic (TM) modes for a square PhC with $f = 0.35$ is shown in Fig. 3(a). The Bloch waves to compute the eigenfrequencies are expanded by 361 plane waves. The dispersion relation between the eigenfrequency $\omega_n = \omega a/2\pi c = a/\lambda$ and the wave vector $\vec{k}$ also leads to a photonic DOS, which plays a critical role for the understanding of the optical properties of PhC(PhQ)-based LEDs. In reality, LEDs emit over a narrow range of spectrum ($\sim 25\,\text{nm}$). According to the photonic band structures, points of intersection between the emitting center frequency and dispersion curves can indicate the permitted modes of emission for a PhC(PhQ)-based LED. The use of the 2D PhC (PhQ) is to turn a guided mode into a radiative pseudo-guided Bloch mode, lying above the light line of air. The periodicity of the 2D pattern is designed to correlate with the wavelength of the organic active region ($\lambda_g = 530\,\text{nm}$), and it induces the Bragg-diffraction effect for the emitted light. It could be expected that the extraction efficiency increases with the density of the radiation mode. The right diagram in Fig. 3(a) displays the DOS of the dispersion relation that is of relevance to the radiation and waveguide modes in this system. In general, the lattice constant for PhCs is selected on the order of the wavelength of the relevant electromagnetic waves, $a \sim \lambda$. It should be noted that the normalized center frequency $\omega_n = 0.86$ with the maximum M^S (Fig. 3(a)) of the DOS above the light line might agree well with the design parameter of the most efficient light extraction for the radiation. In Figs. 3(b) and 3(c), the maxima M^T and M^A can also be obtained for the triangular PhC with $f = 0.3$ and the $(4, 8^2)$ Archimedean tiling with $f = 0.36$, respectively. Besides, the effect of the changes on the radius of the cylinders should be estimated to determine a favorable ratio f. Fig. 4 shows the ratio f dependence of the maximum of the DOS from the dispersion diagram and its corresponding eigenfrequency. For the square PhC, the eigenfrequency $\omega_n = 0.86$ related to the designed lattice constant could be determined from the appropriate ratio $f = 0.35$ which corresponds to the largest

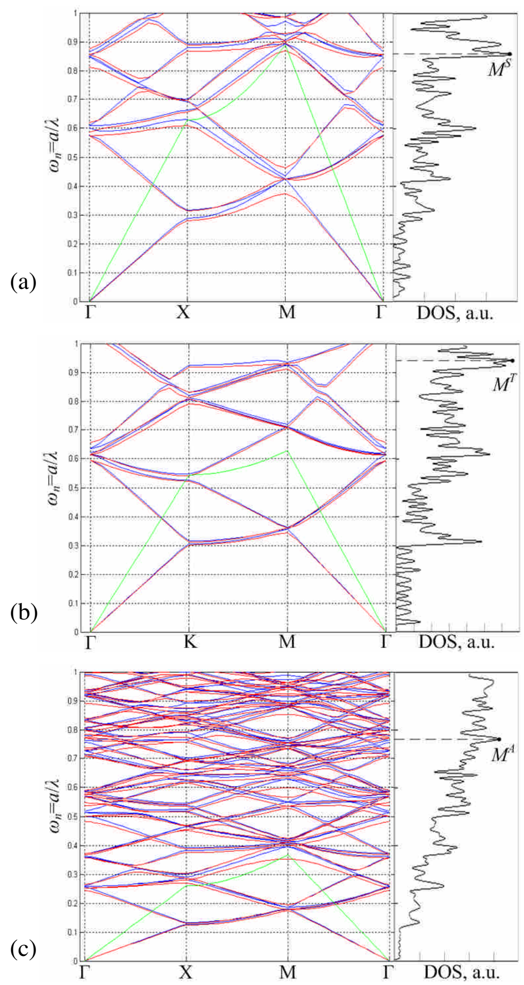

Figure 3. Left: band diagrams of the PhCs constructed from the three kinds of lattice patterns in Fig. 1. Both TE (blue lines) and TM (red lines) polarizations are considered. Green lines indicate the light line. Right: DOS calculated for the corresponding lattice types. The ratio of cylinder radius and lattice constant used for these photonic structures is (a) square: $f = 0.35$, (b) triangular: $f = 0.3$, and (c) Archimedean: $f = 0.36$. M^S, M^T, and M^A indicate the maxima of the DOS in the dispersion diagrams, and their superscripts denote the three kinds of lattices.

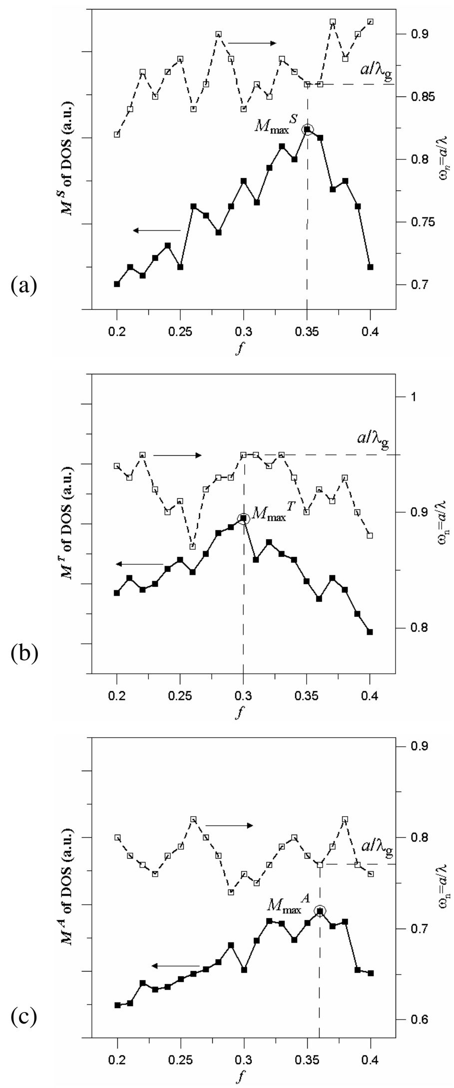

Figure 4. Dependence of the maxima of the DOS and their corresponding eigenfrequencies ($\omega_n = a/\lambda$) on the ratio of cylinder radius and lattice constant, obtained from the dispersion diagrams of the square (a), triangular (b), and Archimedean (c) lattices. $M^S_{\max}$, $M^T_{\max}$, and $M^A_{\max}$ represent the largest values among all maxima of the DOS for the three kinds of lattice patterns, respectively.

value $M_{\max}^S$ among all maxima M^S in Fig. 4(a). The eigenfrequencies given by $\omega_n = 0.95$ and 0.77 corresponding to the largest values $M_{\max}^T$ and $M_{\max}^A$ at $f = 0.3$ and 0.36 can be obtained in the same way for the triangular PhC and the Archimedean PhC in Figs. 4(b) and 4(c), respectively.

The procedures for design and optimization of the PhC (PhQ) structure are summarized as follows:

(1) The selection of the dielectric constants ($\varepsilon_H = n_H^2$, $\varepsilon_L = n_L^2$) to the constituted materials.

(2) The choice of the lattice types.

(3) Establish the dispersion characteristics for an initial ratio $f = r/a$, and calculate the DOS to find its maximum M for the radiation modes above the light line.

(4) Vary the ratio f, and trace the maximum M of the DOS to get a moderate ratio f which gives the largest value $M_{\max}$ and the corresponding eigenfrequency ω_n.

(5) From this eigenfrequency $\omega_n = a/\lambda$, an optimized lattice constant a could be designed to match the desired emission wavelength λ.

Thus, a significant improvement in the light extraction efficiency of the PhC(PhQ)-based LEDs should be expected under the optimized parameters, such as the lattice constant and the ratio of cylinder radius and lattice constant.

4. IMPROVEMENT OF LIGHT EXTRACTION EFFICIENCY

To verify the analysis in Section 3, the light output of the PhC(PhQ)-based LED is calculated by the 3D FEM (COMSOL). The light output is represented by the vertical component of the Poynting vector integrated over the top surface of the simulation domain. The relative extraction efficiency is defined as the fraction of emitted flux through the top surface of the simulation model with the PhC (PhQ) to that without the PhC (PhQ). The full model of the PhC(PhQ)-based LED is shown in Fig. 2. The PhC layer has a thickness of $d = 200$ nm. Via Archimedean tilings with the different ratios f and their corresponding eigenfrequencies ω_n based on the maximum M^A of the DOS. Fig. 5 shows the relative enhancement of the light extraction as a function of the emitting center wavelength λ. The simulation results for theoretical confirmation are to examine the relative extraction efficiency of the LED based on the design procedures of the most effective PhC (PhQ). The relative efficiency of extraction is improved by the introduction of the PhQ. The maximum peaks appear as a result of the light-diffraction effect of the PhQ structure. At the desired emitting wavelength λ_g, it is encouraging to observe the enhancement of ~ 2.8 for an optimized PhQ pattern with a ratio of $f = 0.36$.

For comparison purposes, a plot of the relative extraction efficiency as a function of the emitting center wavelength is presented in Fig. 6 for three kinds of optimized PhC (PhQ) structures shown in Fig. 1. Through the FEM calculation, it is found that the square lattice PhC pattern of $f = 0.35$ registers an enhancement of ~ 1.7 at the emitting center wavelength λ_g. The triangular lattice PhC pattern

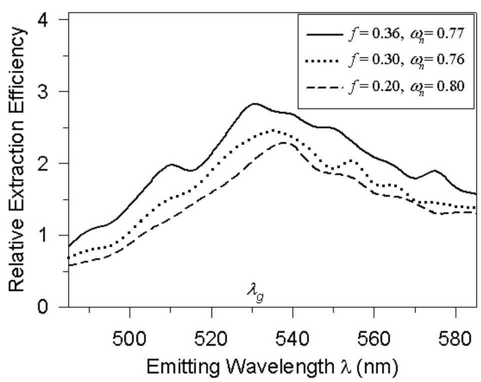

Figure 5. Relative light extraction efficiency versus emitting wavelength under different ratios f and their corresponding eigenfrequencies ω_n for the $(4, 8^2)$ Archimedean tiling of lattice constant $a = \lambda_g \omega_n$.

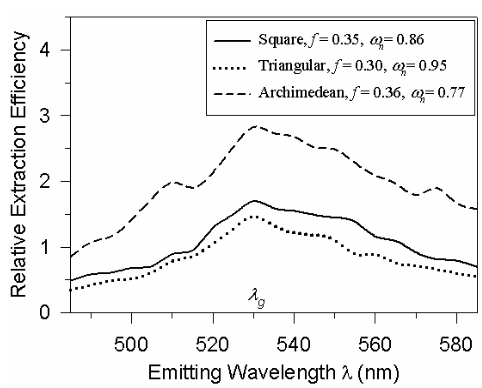

Figure 6. Comparison of relative extraction efficiencies with respect to various emitting wavelengths for the three kinds of lattice patterns with lattice constant $a = \lambda_g \omega_n$.

of $f = 0.3$ shows an enhancement amounting to ~ 1.5. The extraction efficiency of the Archimedean PhC LED is much greater than that of the regular lattice PhC LED. This is attributed to the fact that efficient light collection is achieved when the emitted photons have the energy of a flat band [18]. In the eigenfrequency range adjacent to $\omega_n = a/\lambda_g$, the bands (TE and TM bands) near the Γ point of the reciprocal lattice are relatively flatter in Fig. 3(c) than those in Figs. 3(a) and 3(b). Therefore, as these modes reveal a very low group velocity, photons can couple with the radiation modes after a very low mean free path in the Archimedean PhC structure. In other words, this very high DOS near the Γ point enhances the coupling of emitting photons Nevertheless, the situation is not suitable for the triangular lattice near the Γ point so that the extraction efficiency for this kind of lattice is the lowest.

The thickness of a PhC (PhQ) layer plays an important role in determining the efficiency of cross-coupling between the trapped modes and the radiation modes. For distinct thicknesses d of Archimedean PhC slabs, Fig. 7 shows the extraction efficiency of light under different emitting center wavelengths. The relative extraction efficiency increases with the pattern thickness. Shallow PhQ structures only allow cross coupling between a few higher order trapped slab modes and the leaky PhQ Bloch modes. As depicted in Fig. 7, the extraction efficiency at the specified emitting wavelength (λ_g) increases by up to ~ 3 times for an optimized PhQ pattern with a thickness of $d = 250$ nm and a ratio of $f = 0.36$. Due to practical problems involved in etching very deep holes in the substrate, PhCs (PhQs) will work inherently better with thin LEDs.

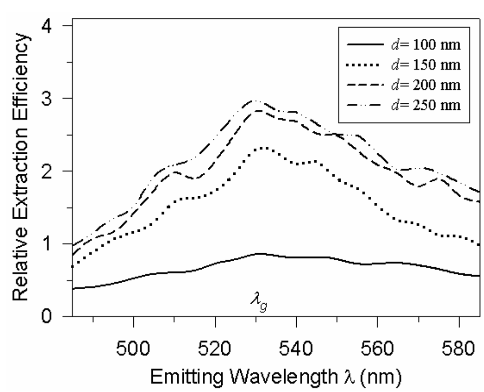

Figure 7. Relative enhancement of extraction efficiency as a function of emitting wavelength for four thicknesses of the Archimedean PhC slab with lattice constant $a = \lambda_g\omega_n$.

5. CONCLUSIONS

Several factors concerning the optimized design of PhC(PhQ)-based LEDs and their effect on the enhancement of light extraction have been discussed. These include the lattice types, the ratio of cylinder radius and lattice constant, the DOS from a dispersion relation, the thickness of a PhC (PhQ) layer, and the position in which a PhC (PhQ) could be inserted. Some rules of practical implementation are offered for high-efficiency LEDs. Benefits of Archimedean tilings known as PhQs were presented, and numerical quantitative comparisons in the relative enhancement of the light extraction based on the 3D FEM were drawn with optimized parameters of improving extraction efficiency. With the use of an optimized periodic pattern of the $(4, 8^2)$ Archimedean lattice, an increase of ~ 2.8 in the extraction efficiency of the LED is expected theoretically. The light extraction for the incorporation of the Archimedean lattice under the optimized parameters exhibits about 1.6 and 1.9 times higher extraction than that of the square and triangular lattices, respectively. The Archimedean tiling pattern provides a favorable consideration of 2D-PhC in light extraction from LEDs.

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