

## LOCAL DISPERSION OF GUIDING MODES IN PHOTONIC CRYSTAL WAVEGUIDE INTERFACES AND HETERO-STRUCTURES

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**Abstract**—Recently, we have introduced a numerical method for calculating local dispersion of arbitrary shaped optical waveguides, which is based on the Finite-Difference Time-domain and filter diagonalization technique. In this paper we present a study of

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photonic crystal waveguides at interfaces and double hetero-structure waveguides. We have studied the waveguide stretching effect, which is the change in lattice constant of photonic crystals along waveguiding direction. Hybrid modes at photonic crystal heterostructure interfaces are observed, which are the results of superposition of existing modes in adjacent waveguides. The dispersion at the interfaces of a double hetero-structure waveguide tends to the dispersion of outer waveguides. The effective area still holding the dispersion of the middle waveguide is shorter than the geometrical length of the middle waveguide. The results of this study present a clear picture of dispersion at interfaces and the transmission in photonic crystal hetero-structures.

## 1. INTRODUCTION

In the past several years, there have been lots of interest in well-designed Photonic Crystal (PC) structures [1–4], since they can control the propagation and localization of light, and have shown very promising applications as functional photonic devices [5], such as low-threshold lasers [6, 7], channel drop filters [8], and optical sensors. Various PC structures and devices designed around the world are not necessarily embedded in a single crystalline PC structure. Even having a photonic-integrated circuit in a single crystalline PC structure is a challenge. There have been PC interfaces reported with different PC lattices in their vicinity, which are known as PC heterostructure [12, 13]. PC heterostructures consist of concatenations of two or more photonic crystals with different band structures, or guiding frequency range, which can be realized by different refractive indices, lattice periods or lattice types [14].

Double heterostructure waveguides are very promising, as they guide the light in certain frequency ranges while confine it in other ranges. Recently, very high quality factors reported in double heterostructures [12, 15]. It has been experimentally shown by Song et al. [12, 16] that high quality factor can be achieved in double heterostructure cavities. These authors have theoretically described the effect using Plane Wave Expansion (PWE) technique. They have described the photon confinement mechanism by analyzing the imaginary dispersion relations and the mode-gap effect [15]. Since PWE is assumed as a method for studying dispersion in infinite periodic structures, a question arises whether PWE is in principle an appropriate method in studying PC heterostructures? One might even argue that the PWE is not suitable for local study of dispersion in non periodic structures.

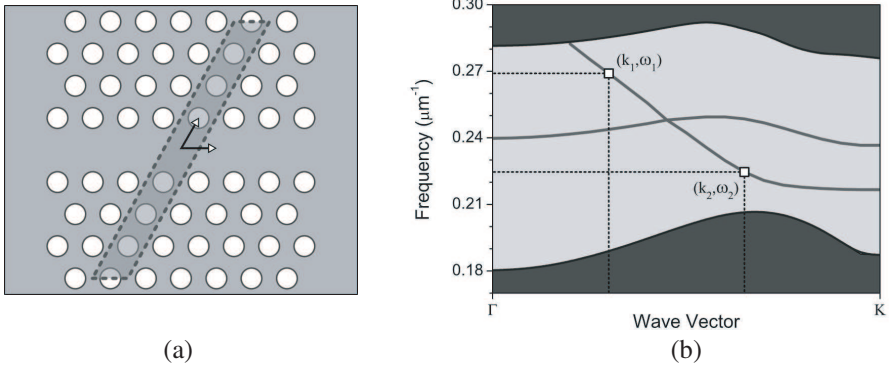
The argument for applying PWE for dispersion calculation in the waveguides is the existence of a short range periodicity, i.e., one can consider that the structure is locally periodic. The assumption of local periodicity is very useful and it can be used to study novel photonic crystal designs including curvilinear and circular PC waveguides [4, 11]. A heterostructure interface, e.g., an interface of two adjacent waveguides, can be an extreme case of non-periodicity, where applying of the PWE is hardly justifiable. The dispersion at a heterostructure interface might not be similar to either of the adjacent waveguides. Generally, the guiding modes of one waveguide might fall into the mode gap of the second waveguide and therefore decay exponentially. Furthermore there might be localized modes at the interface, which decay in both waveguides. The interface states can strongly affect the transmission of light through the structure. It was found that these states can be used to overcome the diffraction limit for light emerging from an aperture of the same size as the wavelength [17, 18].

In this paper, we describe three methods for studying the dispersion: PWE, Spatial Fourier Transform (SFT), and Filter Diagonalization Method (FDM) [20, 21]. We show how the results can be used to study the local dispersion in waveguide interfaces and heterostructures.

## 2. NUMERICAL ANALYSIS OF LOCAL DISPERSION

In order to study the dispersion of photonic crystal waveguides, the PWE method can be applied on a super cell. The super cell is usually a single periodicity cut of the waveguide along the propagation direction and includes several periods in perpendicular direction. The size of super cell along the perpendicular direction should be large enough in order to guarantee that the coupling between artificial neighboring super cells is negligible. Figure 1(a) shows an example of a W1 photonic crystal waveguide in hexagonal array of 2DPCs, consisting of the air holes in silicon background with refractive index of 3.4, and radius of holes is  $r = 0.297a$ . The indicated arrows show the primitive vectors and the parallelogram shows the super cell for PWE calculations. Figure 1(b) shows the dispersion relation for the guiding modes, and the dark color shows areas out of the band gap. We also indicate two points on the guiding mode, with different frequencies  $\omega_1$  and  $\omega_2$ , with corresponding wave vectors  $k_1$  and  $k_2$  for further discussions.

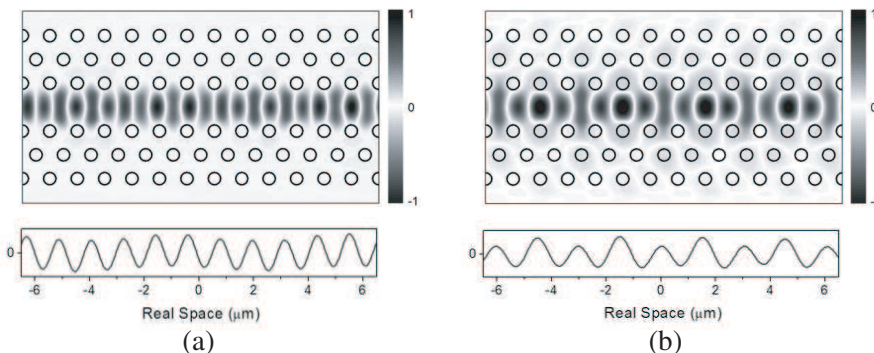
The dispersion relation  $\omega(k)$  holds information about the periodicity of the guiding modes along the propagation direction, and it can be compared with the mode profiles calculated by finite



**Figure 1.** (a) Top view of a W1PC waveguide. The indicated arrows show the primitive vectors and the parallelogram shows the super cell for PWE calculations. (b) Dispersion relation for the guiding modes calculated for  $H$ -polarization. The dark areas indicate the regions out of the band gap. Two indicated points on the guiding mode will be discussed further.

difference time domain (FDTD). Figure 2 shows the modes profile of two frequencies on the guiding mode, indicated in Figure 1(b), and the corresponding cross sections along the propagation direction. The periodicity of these modes along the propagation direction is known as the spatial wavelength  $\Lambda = 2\pi/k$ , where  $k$  is the wave vector. Alternatively, one can extract the  $k$  vectors of an arbitrary waveguide by analyzing the mode profile. In the SFT method, one takes a snapshot of the field along the propagation direction, usually known as window, and performs a signal processing analysis on it. It includes the multiplication of the sampling values with a window function and Fourier transform of it. The results are the spatial frequencies, which describe the number of peaks per unit length along the propagation direction.

One can repeat the procedure over a desired frequency range to extract the dispersion relation of the waveguiding mode. In our previous work [19], we have shown that the SFT results are well comparable with PWE, especially for large window sizes. It is also possible to use windowing techniques to enhance the accuracy of the results. An Alternative approach is to use a filtering technique, as it is well-known in digital signal processing. The filtering technique is one of the common processing approaches which is used in both time and space domain for enhancement of signals. We have considered the Filter diagonalization method and have proven that



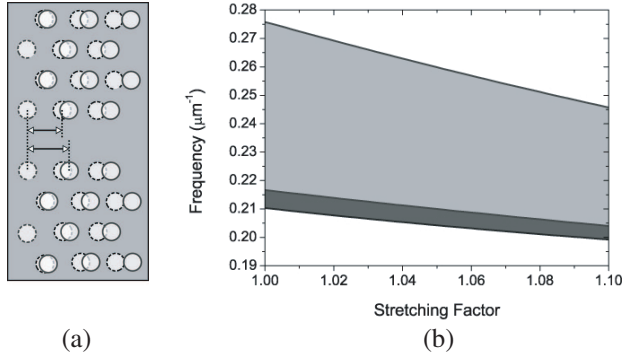
**Figure 2.** Mode profiles of two indicated points in Figure 1(b) with corresponding frequencies of (a)  $\omega_1 = 0.27 \mu\text{m}^{-1}$  and (b)  $\omega_2 = 0.225 \mu\text{m}^{-1}$ . For better comparison, the cross section along the propagation direction is plotted for each mode profile.

the method is very efficient for small window sizes and can be applied to arbitrary waveguides, e.g., curvilinear photonic crystal waveguides [19]. The important assumption in FDM technique is that the field can be written as a sum of exponentially decaying terms  $E(x) = \sum_n a_n \exp(-ik_n x)$ , where amplitudes,  $a_j$ , and complex spatial frequencies,  $k$ , of electromagnetic field over a short spatial window sizes are unknown. The negative imaginary part of  $k$  characterizes the decay rate of the signal.

For both SFT and FDM methods, the FDTD calculation is the most time-consuming part. For very good result with high spatial resolution, the FDTD simulations need to be carried out for tens of hours. An alternative method is to use the Multiple Multipole Expansion (MME) to calculate the stationary field profile and the local density of states [11, 20], however this is not the focus of this paper.

### 3. EFFECT OF STRETCHING ON BAND GAP AND THE WAVEGUIDING MODES

The structural properties of Photonic heterostructures are determined by the lattice parameter mismatch, which we refer as stretching effect. In the heterostructure waveguides designing it is known as a degree of freedom for the optimizing procedures. Song et al. employed the stretching of the PC waveguides in order to design a PC double heterostructure and described the mechanism based on the PWE. They have connected a triangular lattice PC to a deformed



**Figure 3.** (a) Top view of a PC waveguide stretched along  $x$ -direction. The dashed circles represent the un-stretched PC ( $s = 1$ ) and solid circles indicate a PC structure with a stretching factor of  $s = 1.2$ . (b) Mode gap (dark area) and mode guiding (light area) regions as a function of stretching factor.

triangular-lattice structure, which has a larger lattice constant along the propagation direction, while retaining the lattice constant in perpendicular direction, in order to satisfy lattice matching conditions. Here we study the effect of stretching on band gap more in details, by continuously varying the stretching factor.

The stretching factor can be defined as change of horizontal distance between the lenses, while keeping the vertical distance constant. Figure 3(a) shows a W1-PC waveguide stretched by a factor of  $s = 1.2$ . Assuming that the stretched waveguide is infinite, one can still calculate the band gap range and the guiding mode, as it is shown in Figure 3(b). This arrangement consists of air holes in silicon background with refractive index of 3.4, and the radius  $r = 0.297a$ , where  $a$  is the period. The stretching factor increase the lateral distance between neighboring rods along  $x$  direction from 0 to 10 percent.

Figure 3(b) shows the reduction of guiding region with stretching, whereas the mode gap range stays unchanged. In fact due to the stretching the modes with higher frequency, which are out of the band gap range shift down toward the band gap, and reduce the band gap range. The mode gap range, which is shown in dark orange, is the region in which propagation is inhibited.

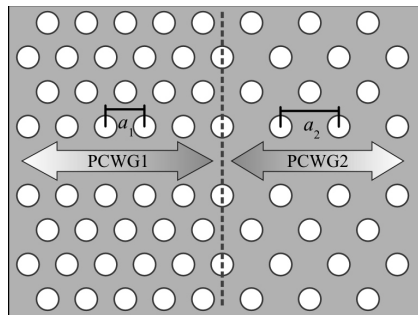
In the rest of this study we will use the same lattice contents which are use by Song et al. and study the local dispersion relation of heterostructure waveguide.

#### 4. LOCAL DISPERSION IN PHOTONIC CRYSTAL WAVEGUIDE INTERFACES

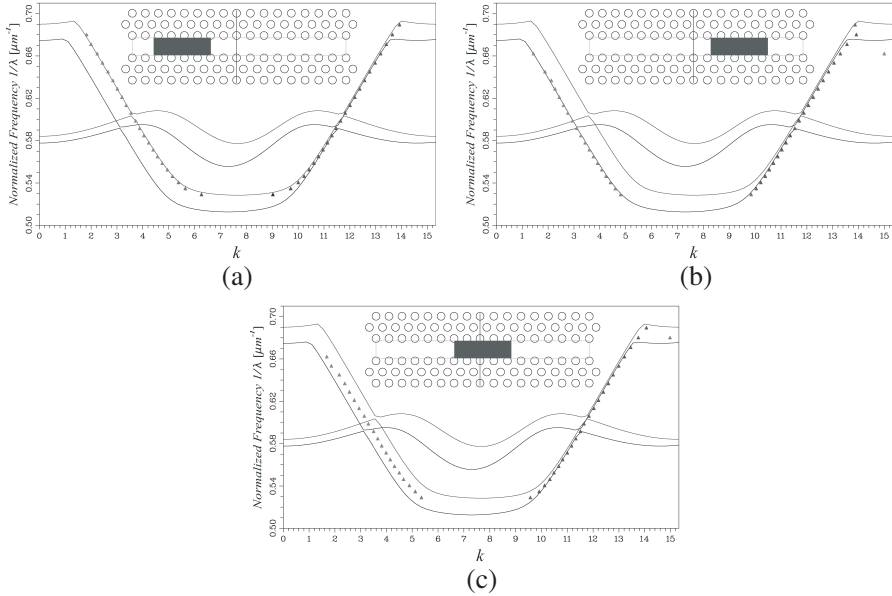
Interface states are states bounded to the interface between two semi-infinite materials, which usually decay exponentially in both of these materials. Interface states can strongly affect the transmission of light between two media. Nevertheless, these bound states do not necessarily appear for all surface terminations, but at least will appear at some cases [21]. The PC heterostructure, which we study in this paper is very similar to the one studied by Song et al. consisting of two PC waveguides, one stretched by a small amount along the waveguiding direction [12]. As it is shown in Figure 4, the structure consists of a W1 PC waveguide in a triangular lattice of air holes in silicon. The left waveguide with the horizontal periodicity of  $a_1 = 0.41 \mu\text{m}$  is connected to the right one, which has the horizontal periodicity of  $a_2 = 0.43 \mu\text{m}$ . In both structures the air holes have radius of  $r = 0.1218 \mu\text{m}$ .

We have presented a novel method to calculate the local dispersion relation in arbitrary photonic crystal waveguides, which is more suitable for local study of dispersion and the special cases of non periodic and finite waveguides. The method is based on the finite difference time domain simulation and Filter Diagonalization Method (FDM), and the accuracy of the results for local studies is much better than Spatial Fourier Transform (SFT), which simply uses the Fourier transform. Generally, numerical methods for study of arbitrary photonic structures which are commonly applied are either PWE or Transfer Matrix Method (TMM), none of which are suitable for study of PC interfaces.

Here, FDM approach is applied to study the dispersion of butt-joint waveguide shown in Figure 4. The scattered data points in



**Figure 4.** Schematic view of two butt-joint waveguides forming a heterostructure with different periodicities  $a_1$  and  $a_2$ .

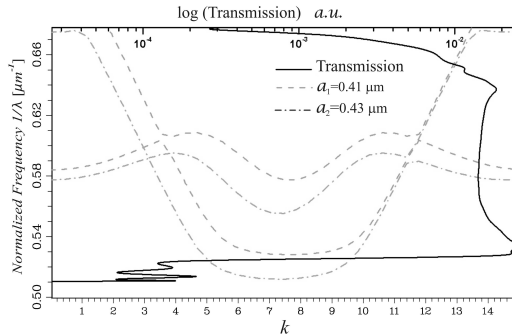


**Figure 5.** Comparison of PWE (solid lines) and FDM results (symbols) for the PC heterostructure at the (a) left waveguide, (b) the right waveguide and (c) the interface of both waveguides. The dark rectangles in the schematic insets show the windows in which the local dispersions are calculated.

Figure 5 show the local dispersion relation at three positions of the butt-joint waveguide. These data points are comparable with PWE calculation of individual waveguides, shown as solid lines. Note that the dispersion relations of the heterostructure are shown without folding because of different periodicity of two waveguide structures, and thus different sizes of the 1st Brillouin zone. The local dispersion relation was calculated over the three windows depicted as black rectangles in the inset of Figure 5. The window size is about 4 times the period of the PC waveguide; therefore the calculated dispersion can be fairly called as local dispersion.

As it is shown in Figure 5, if the window is fully within one of the PC waveguides, the local dispersion calculated by FDM method is in quite good agreement with the corresponding dispersion calculated by PWE. By moving the window toward the interface, the local dispersion calculated by FDM stays single mode, but does not fit to any of two PWE dispersions. Surprisingly, the local dispersion at interface lies on the middle of two PWE dispersion curves. We describe this





**Figure 6.** Dispersion relations of hexagonal PC structures with horizontal period of  $0.41 \mu\text{m}$  (dash line) and  $0.43 \mu\text{m}$  (dash-dot line). The period along the second primitive vector is identical for both structures and equals to  $0.41 \mu\text{m}$ . The solid curve represents the transmission through the hetero-structure.

mode as a hybrid mode which is formed at the interface as a result of superposition of existing modes in adjacent waveguides.

Another important characteristic of an interface is the transmission properties. In order to calculate the transmission diagram, we have used a pulsed source centered at the frequency  $1/\lambda = 0.58 \mu\text{m}^{-1}$ . We can see a large transmission for the frequencies in the range of  $0.525 \mu\text{m}^{-1}$  to  $0.685 \mu\text{m}^{-1}$ , which is the common waveguiding range in two waveguides. On the other hand, there is a dramatic drop by a factor of 100 where the frequency falls into the mode gaps. This is an expected consequence of reflection by one of the waveguides, while the other one still guides the wave.

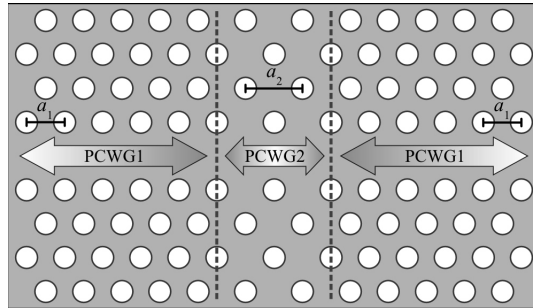
### 5. LOCAL DISPERSION IN PHOTONIC CRYSTAL DOUBLE-HETEROSTRUCTURES

It has been found that the confinement mechanism in double heterostructures is slightly different from that of PC cavities. The abrupt change in the electric field, which happens at the edges of PC cavities, results in significant leaky components. The resulting leakage in out of plane direction does not satisfy the conditions of total internal reflection, which results in low cavity Q factors. Generally, cavities with smooth electric-field distributions have less leaky components, which result is higher Q factors. In order to improve the confinement in PC cavities and optimize the PC structure, one can use a PC double-heterostructure waveguide. The confinement mechanism of the field in

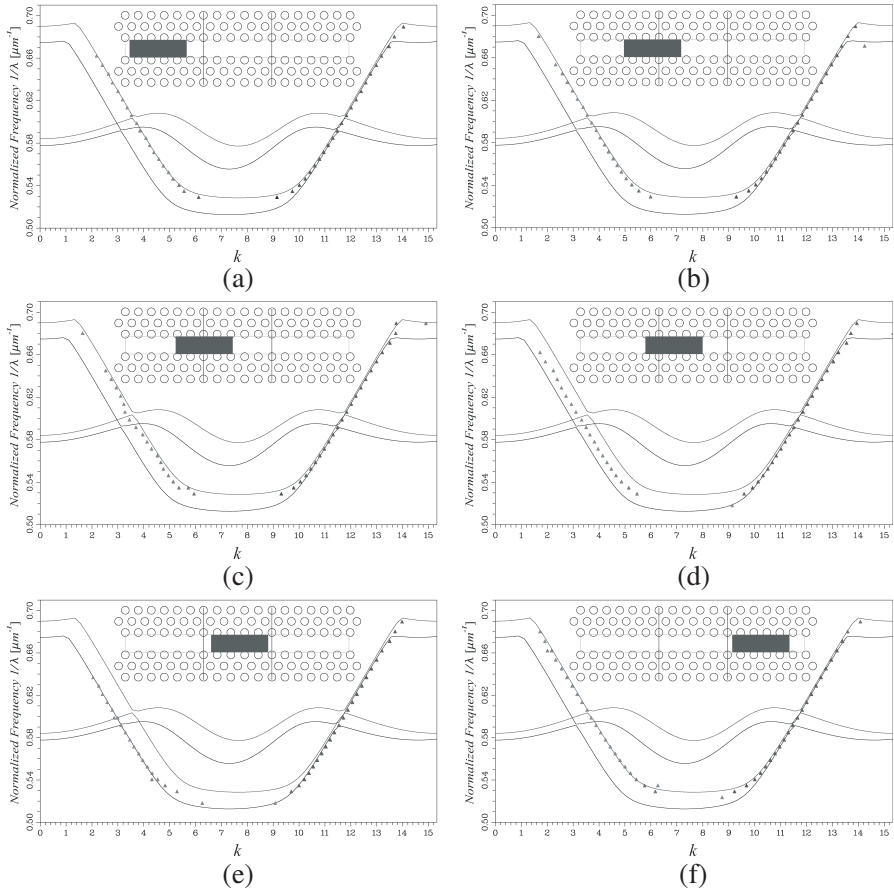
double-heterostructure cavities along the waveguide is based on the mode-gap effect [8, 12]. Investigation of the field profile in double-heterostructures show that the field distribution can be well fitted to a Gaussian function which results in a higher Q factor in the cavity. The discussion about Q factor is out of the scope of this paper, and it is well studied in literature [12].

In recent studies, the PWE method is used to investigate the mode-gap effect [12]. An important point which has not yet been considered is that the PWE is only valid for infinitely periodic structures, although in some studies it is applied to investigate the dispersion in non-periodic arrangements [12]. In DHS waveguides, the periodicity is broken along the waveguiding direction. Regarding to the fact that the dispersion relation is not a quantity to be changed abruptly at the interface, one can not simply adjoin two different dispersions to describe an interface. Nevertheless, the analogy described by Song et al. can describe the localization mechanism to a large extends.

Here we have used the FDM method to calculate the local dispersion at various positions of a DHS shown in Figure 7. The DHS consists of a W1 PC waveguide with horizontal periodicity of  $a_2 = 0.43 \mu\text{m}$ , sandwiched between two W1 PC waveguides with horizontal periodicity of  $a_1 = 0.41 \mu\text{m}$ . The air holes have a constant radius of  $r = 0.1218 \mu\text{m}$ . The procedures of dispersion calculation by PWE and local dispersion calculation by FDM are similar to those we already discussed in previous section. Selected results of the local dispersion calculation at several locations are shown in Figure 8. As we can see in Figures 8(a), (e), (f), if the window is fully inside one of the PC waveguides, the local dispersion calculated by FDM method is



**Figure 7.** Schematic view of a double heterostructure consists of a waveguide of periodicity  $a_2$  sandwiched between two waveguides of periodicity  $a_1$ .



**Figure 8.** Local dispersion relation and comparison with PWE results. The window is located at different position, indicated with rectangle, moving along PC waveguide double heterostructures. The dark rectangle in the schematic insets shows the window in which the local dispersion is calculated.

in a very good agreement with the corresponding dispersion calculated by PWE. Similar to the heterostructure studied earlier, by moving the window toward the interface, the local dispersion stays single mode, however it neither fits to any of the two PWE dispersions, nor falls in the middle of the dispersion of neighboring waveguides. As it is seen in Figure 8(c), the dispersion of a DHS waveguide calculated on a window located exactly at the interface, tends to the dispersion

of outer waveguides. One can argue that the guiding mode at this interface gets a stronger influence from the outer waveguides than the middle waveguide. In fact the effective area still holding the dispersion of middle waveguide is only about  $3 \times a_2$ , which is shorter than the geometrical length of the waveguide that is  $5 \times a_2$ .

## 6. CONCLUSION

We studied the stretching effect, which increases the distance between neighboring rods along the guiding direction of PC waveguides. By continuously changing the stretching factor, we observed that the band gap and guiding region shorten in frequency, while the mode gap width remains unchanged. By connecting two waveguides with different stretching factors, we arranged a PC waveguide interface or so-called PC heterostructure.

We studied the local dispersion properties of a PC interface and a double hetero-structure waveguide by applying two different methods. We have applied FDM method to the field distribution snapshots of the FDTD simulations to study the local dispersion relation of hetero- and double hetero-structure waveguides. The dispersion relation results were compared with those calculated by the standard PWE technique. It is described that PWE uses an assumption of infinite waveguides. Therefore, it is not suitable for describing the dispersion at the interface, since interface modes are not similar to any of the adjacent waveguiding modes.

We have also studied the local dispersion relation in the double-hetero-structure waveguide previously reported by Song et al. The local dispersion results of the FDM method show a smooth switching between the modes of two different structures. The dispersion at the interfaces of a double hetero-structure waveguide tends to the dispersion of outer waveguides. The effective area still holding the dispersion of the middle waveguide is shorter than the geometrical length of the middle waveguide. The results of this study provide new insight into study local dispersion in any arbitrary photonic interface or double heterostructure.

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