Influence of surface termination on inverse Goos–Hänchen shift of negatively refractive photonic crystals

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Abstract
The effect of surface termination on the inverse Goos–Hänchen (GH) shift of two-dimensional (2D) negatively refractive photonic crystals (NRPhCs) containing air holes arranged in a hexagonal lattice in a dielectric background is investigated for transverse magnetic (TM) polarization. Results show that the magnitude of the inverse GH shift of 2D-NRPhCs strongly depends on surface termination even for an incident beam with a fixed frequency and incidence angle. Calculation of dispersion of surface mode as a function of termination reveals that large inverse GH shift of 2D-NRPhCs results from the excitation of backward surface mode. In addition, the coupling coefficient of the incident field into the field of surface mode and energy flux around the interface are studied and demonstrate the above conclusion. This paper will provide technical information regarding the combination of various functional photonic elements in the design of integrated optical circuits.

Keywords: surface termination, Goos–Hänchen effect, negative index, photonic crystals

(Some figures may appear in colour only in the online journal)

1. Introduction

Light reflection and refraction at a plane dielectric interface is one of the most basic optical phenomenon and is present in practically all optical systems. Especially, when a bounded wave beam is incident at critical angle, from an optically more dense medium to a less dense medium, total reflection occurs, which is accompanied by a sizable lateral shift of the center of reflected beam from the position predicted by geometrical optics, and the lateral shift is named the Goos–Hänchen (GH) shift [1] in memory of the first measurement of this tiny lateral shift. The GH shift occurs as a result of the different phase acquisition of the plane wave components of the finite incident beam and is given as $S = -d\phi/kd\theta$ [2], $\phi$ is the phase of reflected beam, $k$ and $\theta$ are the wave vector number and the incidence angle, respectively, in the incident medium. In most situations, the GH shift is positive, that is, the GH shift is in the opposite side of the normal from the incident beam. Most recently, the interest in the study of GH shift renews due to the realization of materials with negative index of refraction, such as left-handed materials (LHMs) [3], negatively refractive photonic crystals (NRPhCs) [4, 5], and the prediction of Veselago [6] that electromagnetic waves traveling through materials with negative index of refraction would result in opposite effects, such as reversed Doppler effect, and reversed Vavilov–Cerenkov effect. According to Veselago’s deduction, inverse GH shifts will occur at the interface of materials with the opposite sign of refractive index when total reflection takes place. In this paper, we mostly focus on the inverse GH shift of NRPhCs.
It has been reported in papers [7, 8] that photonic crystals (PhCs) under certain conditions can behave with refraction as obeying Snell’s law with a negative effective phase index $n_{\text{eff}} < 1$. Thus, a wave propagating from air to the PhCs is essentially a wave coming from an optically more dense medium to a less dense medium; hence inverse GH shift will take place when the incidence angle is equal to or even above the critical angle. Inverse GH shift of NRPhCs has been theoretically discussed by He et al [9], in which giant inverse GH shift was obtained by adding an homogeneous cladding layer of appropriate thickness between air and the NRPhCs. However, the influence of surface termination of NRPhCs on the inverse GH shift has not been taken into account. In fact, the physics of GH shift in PhCs is a bit intricate due to the remarkable surface effect, because PhCs are a periodic medium and the modes repeat periodically in the reciprocal space.

This paper aims to investigate the influence of surface termination on the inverse GH shift of NRPhCs. To the best of our knowledge, no study has focused on this problem but a few works have investigated the effect of surface termination on the optical properties of PhCs. Previous studies have investigated the role of surface termination on the reflection and transmission spectra of 2D-PhCs; results have demonstrated that surface termination generates dips within the photonic stop bands of the reflection spectra in TM and TE polarizations [10, 11]. Lu et al [12] reported that electromagnetic waves can be guided at the edge of three-dimensional PhCs in air by using a specific design of the intersection of two-surface planes. Another study has demonstrated that the beam direction from a PhCs waveguide can be controlled by changing its surface termination [13].

In the present paper we choose the structure with hexagonal air holes in dielectric slab as the 2D-NRPhCs because such structure can be easily fabricated with negative effective index $n_{\text{eff}} < 1$ in the second band for TM polarization [8]. By changing surface termination (position of surface plane) we calculate the inverse GH shift of 2D-NRPhCs as a function of surface termination. Then, the dispersion of surface mode as a function of surface termination is given to explore the origin of the effect of surface termination on inverse GH shift. Last, by introducing the coupling coefficient of the incident field into the field of surface mode the characteristic of inverse GH shift is well explained, and energy flux at the air-NRPhCs interface confirms the conclusion.

In our calculation the plane wave expansion method (PWEM) [14] is used to obtain the frequency band structure and the equifrequency surface (EFS) of PhCs. And the supercell method [15] based on PWEM is used to get the dispersion of surface mode (as a function of surface termination) by applying the Bloch theorem. To get the curve of inverse GH shift of 2D-NRPhCs as a function of surface termination we used commercial software FDTD Solution with the boundary condition of PML [16] to simulate the reflection of bounded wave beam at the interface of air and NRPhCs, and monitored the profile of the reflected beam. Then, the magnitude of inverse GH shift is extracted by obtaining the horizontal coordinate of the maximum value of reflected beam [17].

2. Structure

We consider 2D-PhCs, which consist of hexagonal lattice of air holes in a dielectric background with dielectric constant of 12.96 (e.g., GaAs at the near infrared region). The radius of air holes $r = 0.4a$, where $a$ is the lattice constant. Here, we only take into account TM polarization. The $xz$ plane is set as the plane of periodicity, which is parallel to the propagation vector. The interface between air and 2D-PhCs is parallel to the $\Gamma - K$ direction.

There are two prerequisites that should be satisfied for designing PhCs with negative index of refraction [18]. First, the slope of band curve should be negative, meaning that the angle between the direction of group velocity and that of phase velocity is obtuse, i.e., $v_g \cdot k < 0$. It has been proven analytically [19] that for an infinite PhCs system the group velocity has the same direction as the energy velocity, i.e., Poynting vector $p$. Therefore, the sign of $v_g \cdot k$ is equivalent to the sign of $p \cdot k$, and the sign of $n_g$ is same as the sign of $v_g \cdot k$. Readers who want to know more about group index, phase index, group velocity and phase velocity can refer to [20]. Second, the band curve should be as symmetrical about $\Gamma$ as possible, implying that the equifrequency contour (EFC) of this band is almost circular. Then, the PhCs in the corresponding frequency region can be taken as isotropic material. With this in mind, we plot the first four bands of TM polarization (in figure 1(a)) and find that the second band (denoted as bold blue curve) satisfies the two prerequisites. Then, we plot the EFC of the second band curve in figure 1(b). The hexagon composed by dotted lines is the 1st Brillouin zone (BZ). It is apparent that the EFC in the normalized frequency region from 0.3–0.34 $\omega a/2\pi c$ are circular, and the EFC shrinks with increase of frequency, i.e., $v_g \cdot k < 0$. Thus, the PhCs in this frequency region can be considered as isotropic material with negative index of refraction. In other words, light propagating in these PhCs has the characteristic of opposite sign between the direction of group velocity and that of phase velocity. Here, we plot in figure 2 the directions of group and phase velocities in PhCs by means of Huygens principle [21] when a beam of 0.33 $\omega a/2\pi c$ illuminates the surface of PhCs from the air side. From these EFC the effective phase index of PhCs can be calculated as the ratio of the radii of EFC of PhCs (red circle) and air (blue circle) [18], i.e., $n_p = -0.485$, corresponding to critical angle 29 deg. In figure 2(a), the beam with normalized frequency of 0.33 is incident from air (left region) onto the surface (denoted by the black vertical dotted line) of PhCs (right region) at critical angle, as shown by the blue arrow. The brown horizontal dotted line denotes the conserved k line as well as the normal of the surface. It is apparent that the group velocity (represented by the green arrow) in PhCs is opposite to the phase velocity (shown by the red arrow). What is more, the group velocity is along the surface of PhCs, i.e., total reflection takes place. For an incidence angle above critical angle, total reflection takes place, and inverse GH shift is possible. Note that to obtain one reflected and/or refracted beam, the neighboring equifrequency circles should not
intersect with the conserved k line \([20]\), as the situation shown in figure 2(b).

### 3. Results and discussion

He et al [9] reported that total reflection at the interface between NRPhCs and air is accompanied with inverse GH shift, which can be enhanced by adding a homogeneous cladding layer with appropriate thickness. However, the effect of surface termination on inverse GH shift of NRPhCs has not been studied. Here, we report theoretically that the inverse GH shift of NRPhCs is strongly influenced by the surface termination of NRPhCs and can also be enlarged when NRPhCs’ surface is terminated at a reasonable position. The results are obtained by means of commercial software FDTD Solution. First of all, we introduce the termination parameter \(\tau\) \((0 \leq \tau < 1)\), which corresponds to the length of the unit cell in the \(z\) direction (i.e., 0.866\(a\)) and linearly increases with increasing the height of the surface. When \(\tau = 0\), the outermost row of air holes exhibit a complete profile (i.e., perfect termination, as shown in the inset of figure 3). The incident beam used to illuminate the interface of air and 2D-NRPhCs has width of 16\(a\) with Gaussian profile in its cross-section. The result is presented in figure 3, in which the horizontal axis is the termination parameter \(\tau\) and the vertical axis is the inverse GH shift. As expected, when total reflection occurs at the interface between air and NRPhCs, inverse GH shift is

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**Figure 1.** (a) Band diagram of 2D-PhCs with hexagonal lattice of air holes in dielectric slab, \(\varepsilon_{slab} = 12.96\), \(\varepsilon_{air} = 1\). The radius of air holes \(r = 0.4a\), where \(a\) is the lattice constant. \(M\), \(\Gamma\), \(K\) are the high symmetrical points of 1st BZ and \(\Gamma\) is the center of 1st BZ. (b) The EFC of the second band (bold blue circle in figure 1(a)) in the 1st BZ (the dotted hexagon), the frequencies are uniform between 0.3–0.34 \(\omega a/2\pi c\) from the outermost circle to the innermost one.

**Figure 2.** The directions of group (denoted by green arrow) and phase (denoted by red arrow) velocities in (a) 1st BZ and (b) repeated BZ for reflection of TM polarization with normalized frequency 0.33 at the air-NRPhCs interface (denoted by black vertical dotted line). The blue and red circles are the equifrequency contour of air and PhCs, respectively. The beam (denoted by blue arrow) is incident from air (left region) onto the surface of NRPhCs (right region) at (a) 29 deg and (b) 30 deg. The brown horizontal dotted line is the conserved k line and the normal of the interface as well.
and corresponds to the length of a unit cell in the $z$ direction. The inset shows the situation of $\tau = 0$ and 0.5.

Figure 3. The curve of inverse GH shift of 2D-NRPhCs as a function of surface termination $\tau$ for TM-polarized beam incident at critical angle 29 deg. The interval $0 \leq \tau < 1$ corresponds to the length of unit cell in the $z$ direction. The inset shows the situation of $\tau = 0$ and 0.5.

observed. Unlike the normal GH shift of totally internal reflection of isotropic homogeneous materials, however, the inverse GH shift remains not constant on the condition that the beam is incident at critical angle; on the contrary, it is dramatically affected by surface termination. For surface termination $\tau = 0.25$ and $0.85$ or so, the inverse GH shift gets its maximum values, $-28.27 a$ and $-9.215 a$, respectively. For other surface terminations the inverse GH shift of NRPhCs is very small, even zero.

Previous studies showed that the interface of media always supports surface modes under some condition [22], and this is all the more so for PhCs due to its periodic surface [23], in the same way NRPhCs support backward surface wave [24]. Therefore, the inverse GH shift at the surface of NRPhCs may be associated with its backward surface wave. To investigate the relation between the inverse GH shift and backward surface wave we calculate the dispersion of surface mode as a function of termination $\tau$ with incidence angle fixed at critical angle. Due to the breaking of translational symmetry in the normal direction we must consider a super-cell that spans the entire PhCs slab in the normal direction [15]. This super-cell consists of only one unit cell along the lateral direction, where translational symmetry still applies. Nevertheless, several PhCs sites (including the air region) should be taken along the normal direction. The number of sites, as well as the length of the air space on the top and bottom of the terminated PhCs slab, must be thick enough to disallow any mode coupling between the top and bottom PhCs slab. In our calculation the PhCs slab has the thickness of 51 periods and the thickness of air regions on the top and bottom of the PhCs are 7 periods.

The dispersion of surface mode as a function of surface termination is shown in figure 4, in which the horizontal brown line corresponds to the normalized frequency 0.33. From this figure we can see that the dispersion of surface mode varies with the change of surface termination. In the ranges $0.15 \leq \tau < 0.3$ and $0.7 \leq \tau < 0.9$ the slope of surface dispersion is steep, that is, the surface mode is sensitive to surface termination. Intersects at terminations $\tau = 0.25$ and 0.85 between the horizontal line and dispersion of surface mode reveal that the incidence of TM light with frequency 0.33 can excite backward surface wave of PhCs. Comparing the results to those presented in figure 3, we can conclude that giant inverse GH shift takes place for those terminations where backward surface wave is excited. That is to say, giant inverse GH shift originates from the excitation of backward surface wave of NRPhCs.

As for the descent of dispersion of surface mode with increasing termination, the physical reason may be understood as follows: according to the electromagnetic variational principle [25], the low-frequency modes concentrate their energy in the high-$\varepsilon$ regions, and the high-frequency modes have a larger fraction of their energy in the low-$\varepsilon$ regions. With increase of surface termination, i.e., the augment of high-$\varepsilon$ region, more modes with low frequency are allowed in NRPhCs; while modes with high frequency become less. In other words, with increase of surface termination, modes are pulled down from upper band to lower band, and the slope of surface mode is negative.

One may question why the inverse GH shifts of NRPhCs with terminations $\tau = 0.25$ and 0.85 are not the same now that backward surface modes are excited at these two terminations. To answer this question, we have to quantitatively study the relation between inverse GH shift and surface termination; we cannot obtain the reason from the above researches (e.g., figures 3 and 4) because they are qualitative. Here, we determine the relation between the magnitude of inverse GH shift and surface termination by introducing the wave coupling coefficient of incident field into surface mode of NRPhCs. Generally, the more energy incident field is coupled into the surface wave the larger the magnitude of inverse GH shift. The definition of coupling coefficient is
defined by the following formula [26]:

\[ c = \frac{\langle S_{\text{NRPhC}} \rangle}{\langle S_m \rangle} \]  

where \( \langle S_{\text{NRPhC}} \rangle \) and \( \langle S_m \rangle \) represent the time-averaged power fluxes of the backward surface field in 2D-NRPhCs and the incident field, respectively, within unit cell along the surface. To find a complete description about the definition of coupling coefficient readers can refer to [27, 28].

Figure 5 clearly shows that there are two maxima values for the coupling coefficient at \( \tau = 0.25 \) and 0.85, and the value elsewhere is almost zero. Furthermore, the coupling coefficient of \( \tau = 0.25 \) is much larger than that of \( \tau = 0.85 \); this is the reason that inverse GH shift of \( \tau = 0.25 \) is much larger than that of \( \tau = 0.85 \).

We also plot the energy flux around the interface (i.e., the horizontal red line) between air (i.e., the region below the horizontal red line) and NRPhCs (i.e., the region above the horizontal red line) for terminations \( \tau = 0.25 \) and 0.85 in figures 6 and 7, respectively. The vertical red line is the normal of interface, the intersect point of which with the horizontal red line represents the center of incident beam, which illuminates the interface from the lower left corner. For better visualization only the area \( 3a \times 3a \) around the incident center is presented. From the picture of energy flux, we can clearly see that the backward surface wave (propagating towards left) at the surface of NRPhCs is excited under the illumination of TM beam with frequency of 0.33, and concentrates most of its energy (denoted by red color) in high-\( \varepsilon \) material. Compared to the situation \( \tau = 0.85 \), the energy of backward surface wave for termination \( \tau = 0.25 \) is concentrated much closer to the surface of NRPhCs, which makes the radiation of backward surface wave into air more efficient and gives rise to larger inverse GH shift.

There is one point that should be stressed. Although both giant inverse GH shifts are based on the NRPhCs system, the physical mechanism of the giant inverse GH shift in the paper of He et al [9] is different from this paper. In the paper of He et al, the PhCs system consists of three layers: the air layer, the homogeneous cladding layer and the PhCs. When light is incident on the air-cladding interface satisfying the phase matching condition, the reflected beam has double peaks: the main peak corresponds to giant inverse GH shift, which results from the excitation of backward leaky guided mode in the waveguide, i.e., the homogeneous cladding layer; the small peak corresponds to direct reflection at the air-cladding interface. That is, the giant inverse GH shift results from backward leaky guided mode in the cladding layer. However, the giant inverse GH shift of this paper has given rise to the excitation of backward surface wave at the surface of NRPhCs, which has little to do with the waveguide mode.
4. Conclusion

In conclusion, we have investigated the effect of surface termination on the inverse GH shift of 2D-NRPhCs. Results show that surface termination plays a crucial role in the magnitude of inverse GH shift as well as the excitation of surface wave of 2D-NRPhCs even for a beam with a fixed frequency and incidence angle. Then, study on the dispersion of surface mode of NRPhCs and energy flux around the air-NRPhCs interface suggests that the origin of large inverse GH shift is the excitation of backward surface mode of NRPhCs, which is different from the giant inverse GH shift in [9] where the homogeneous cladding layer is added at the surface of NRPhCs. Last, calculation of the coupling coefficient of incident field into backward surface field demonstrates the above conclusion. The result of this paper will provide technically significant information regarding the combination of various functional photonic elements in the design of integrated optical circuits.

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