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Enhanced and one-way absorptance of LiNiO₂ thin films in one-dimensional photonic crystals

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Abstract

The refractive index of LiNiO₂ thin films is complex and exhibits both dielectric and metallic properties. With LiNiO₂ thin films coated on or inserted in photonic crystals (PCs), it is possible to enhance the absorptance in the designed (AB) n LiNiO₂ (BA) m PC structures. One-way absorption in the photonic bandgap of (AB) PCs has been observed via changing the optical transmitting direction. The positions, width, and strength of the absorption peaks depend on the thickness of the LiNiO₂ films, the incident angles, and the transverse electric/transverse magnetic modes. The photonic band structure can be employed to determine the allowed and forbidden photonic modes and the related optical properties for (AB) PC and (AB) n LiNiO₂ PCs. These novel absorption characteristics can enrich the optoelectric properties of LiNiO₂ thin films.

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Enhanced and one-way absorptance of LiNiO_2 thin films in one-dimensional photonic crystals

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Enhanced and one-way absorptance of LiNiO_2 thin films in one-dimensional photonic crystals

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The refractive index of LiNiO_2 thin films is complex and exhibits both dielectric and metallic properties. With LiNiO_2 thin films coated on or inserted in photonic crystals (PCs), it is possible to enhance the absorptance in the designed $(\text{AB})^n\text{LiNiO}_2(\text{BA})^m$ PC structures. One-way absorption in the photonic bandgap of (AB) PCs has been observed via changing the optical transmitting direction. The positions, width, and strength of the absorption peaks depend on the thickness of the LiNiO_2 films, the incident angles, and the transverse electric/transverse magnetic modes. The photonic band structure can be employed to determine the allowed and forbidden photonic modes and the related optical properties for (AB) PC and $(\text{AB})^n\text{LiNiO}_2$ PCs. These novel absorption characteristics can enrich the optoelectronic properties of LiNiO_2 thin films. *Published by AIP Publishing.*

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I. INTRODUCTION

A photonic crystal (PC) is a periodic arrangement of dielectric elements along some direction, with the distances between the adjacent units of the order of the electromagnetic wavelength of operation.^{1,2} PC related materials and structures exhibit unusual electromagnetic properties not seen in either dielectrics or metals. These properties lead to applications such as photovoltaics,^{3,4} photodetectors,^{5,6} biosensors,^{2,7} and stealth materials.⁸ By controlling and manipulating the flow of light in different wavelength ranges and/or constituting different PC structures with different widths,^{8,9} the reflectance, transmittance, and absorptance can be designed and modified. These properties in PC structures can be understood from the photonic bandgap structure, where photons whose energies lie in certain intervals cannot propagate in any direction.^{10,11}

Light can hardly penetrate bulk metals because of the large negative permittivity but positive permeability where thicknesses are larger than the skin depth. The presence of a metal material in a PC will lead to mode dispersion in the photonic bandgap or gap formation.¹² The enhanced absorption in multilayer metal/dielectric structures has been observed experimentally and theoretically.¹³ When the thickness of a metal material is small enough, some electromagnetic wave can propagate and the one-way absorption behavior of the anti-resonant mode in one-dimensional dielectric/metal PC structures with a dielectric defect layer has been observed.¹⁴ The transmittance of a single metal layer can be enhanced by two orders of magnitude if it is sandwiched between two

dielectric PCs to excite the tunneling modes (or propagation states) within the forbidden gap of the PC for all the angles of optical incidence for both transverse electric (TE) and transverse magnetic (TM) modes.¹²

At present, LiNiO_2 , LiCoO_2 , and related materials have attracted much attention for Li-ion batteries, being considered to be the most promising energy storage devices, for applications such as hybrid electric and pure electric vehicles.^{15–18} Dielectric spectroscopy can be used to analyze the electronic conductivity which is one of the major and important properties in these composite materials.^{18,19} The I - V curves of the field effect transistor device based on Li-NiO nanowires has been investigated experimentally.²⁰ LiMO_2 ($M = \text{Ni, Co, Mn}$) can also be fabricated into thin films. The discharge capacity in a $\text{LiCoO}_2/\text{LiNiO}_2$ multilayer thin film is superior to that of a single layer thin film, which indicates that this multilayer thin film is a good cathode material.²¹ An understanding of optical and transport properties of these materials can facilitate technological applications. El-Bana *et al.* used a conventional pyrolysis technique to synthesize LiNiO_2 thin films with thickness of 200 nm–354 nm.²² The transmittance and reflectance have been investigated, and the wavelength-dependent refractive index and absorption index have been obtained. The LiNiO_2 thin films exhibit both dielectric and metallic properties and can be inserted in or coated on the layered dielectric structures. It is expected that the absorptance increases and the optical transport properties can be modified in the case of multilayer dielectric structures and/or photonic crystals with a metal channel. As in monolayer graphene with novel conductivity, enhanced biosensing and enhanced optical absorption have been obtained in graphene-based 1D PCs.^{7,23}

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This has been designed as a microcavity-integrated graphene photodetector^{24,25} or other graphene devices.²⁶

Motivated by this research, in this paper, the effect of LiNiO₂ thin films on optical properties will be investigated. We present the results of the absorptance as a function of the wavelength (or frequency), TE/TM polarized modes, and the incident angle in the (AB)ⁿLiNiO₂(BA)^m PC structures, where $n, m = 0, 1, 2, \dots$ (A = 1st dielectric material and B = 2nd dielectric material). We analyze the transmittance and the photonic energy band structures calculated by the transfer matrix approach.

II. THEORETICAL APPROACHES

The optical transport properties of a multilayer structure can be investigated using the transfer matrix method. The homogeneous surfaces of layers are located in the x - y plane, and the z -axis is normal to the x - y plane. Taking into account the electric and magnetic boundary conditions, the transfer matrix for the TE mode and TM mode in the j th layer is given as

$$M_j^{TE} = \begin{pmatrix} \cos(k_{z,j}d) & (i/\eta_j^{TE}) \sin(k_{z,j}d) \\ i\eta_j^{TE} \sin(k_{z,j}d) & \cos(k_{z,j}d) \end{pmatrix}, \quad (1)$$

where $\eta_j^{TE} = k_{z,j}/(\omega\mu_i)$, k_z is the wavevector perpendicular to the 2D plane, and

$$M_j^{TM} = \begin{pmatrix} \cos(k_{z,j}d) & -(i/\eta_j^{TM}) \sin(k_{z,j}d) \\ -i\eta_j^{TM} \sin(k_{z,j}d) & \cos(k_{z,j}d) \end{pmatrix}, \quad (2)$$

where $\eta_j^{TM} = k_{z,j}/(\omega\epsilon_i)$. In the presence of the complex refractive index $\tilde{n} = n + i\kappa$, the wavevector along the z -direction can be replaced by a complex function $k_z = \beta_z + i\alpha_z$. The real and imaginary parts represent propagation and attenuation of the electromagnetic wave, respectively, which can be described as $\beta_z = \frac{1}{\sqrt{2}} \left[\sqrt{(k_0^2\epsilon'_r - k_x^2)^2 + (k_0^2\epsilon''_r)^2} + (k_0^2\epsilon'_r - k_x^2) \right]^{1/2}$

FIG. 1. The absorptance as a function of frequency from 30 to 300 THz in (AB)¹⁰D(AB)¹⁰⁻ⁿ with the thickness of 354 nm for LiNiO₂ film at normal incidence. $n = 1, 3, 5, 9$ for the solid (black), dashed (red), dotted (blue), and dashed-dotted (green) lines, respectively. (b) is a zoomed-in view of the resonance absorption regions.

and $\alpha_z = \frac{1}{\sqrt{2}} \left[\sqrt{(k_0^2\epsilon'_r - k_x^2)^2 + (k_0^2\epsilon''_r)^2} - (k_0^2\epsilon'_r - k_x^2) \right]^{1/2}$. k_0 is the vacuum wavevector. $k_x = k_0 \sin \theta_i$ with θ_i being the incident angle. The real ϵ'_r and imaginary ϵ''_r parts of the complex dielectric constants can be written in the form of $\epsilon'_r = n^2 - \kappa^2$ and $\epsilon''_r = 2n\kappa$.

Using the transfer matrix, the electric field E and the magnetic field H in the first and last layers for the TE mode satisfy the following forms:

$$\begin{pmatrix} E_i \\ H_i \end{pmatrix} = M_1^{TE} M_2^{TE} \cdots \begin{pmatrix} E_f \\ H_f \end{pmatrix}. \quad (3)$$

The subscripts i and f indicate the initial and final layer, respectively. Therefore, the reflection (r), transmission (t) coefficients, and the absorptance (A) of LiNiO₂ thin films can be readily obtained using the four elements of the transfer matrix. $E_i = e^{ik_{z,i}d_i} + r e^{-ik_{z,i}d_i}$ for TE mode. r and t are the amplitude ratios of the reflective and transmitted electric (magnetic) field component to the incident component for the TE (TM) mode. d_i is the incident position of the light beam. For the TM wave, two field components of the column vectors are $\begin{pmatrix} H \\ E \end{pmatrix}$. $A = 1 - |r|^2 - \frac{n_f \cos \theta_f}{n_i \cos \theta_i} |t|^2$ and $A = 1 - |r|^2 - \frac{n_i \cos \theta_i}{n_f \cos \theta_f} |t|^2$ for the TE and TM modes, respectively. $|r|^2$ and $\frac{n_i \cos \theta_i}{n_f \cos \theta_f} |t|^2$ represent the associated reflectance and transmittance. Considering the proposed structure of N period of layers and extending the finite layers into the infinite periodic structures (i.e., PC), based on the Bloch's theorem and the boundary condition, the photonic band structure for TE/TM modes can be obtained,

$$\cos(\beta\Lambda) = \frac{1}{2} \text{Tr}(M_1^{TE/TM} M_2^{TE/TM} \cdots). \quad (4)$$

β is the vertical component of the Bloch wavevector. Λ is a periodic thickness of the unit cell. Because of the complex refractive index, the wavevector $\beta = \beta' + i\beta''$. The imaginary part corresponds to the photonic bandgap and the optical absorption.

FIG. 2. The transmittance as a function of frequency in (AB)¹⁰ (black solid line), (AB)¹⁰D (red dashed line), and (BA)¹⁰D (blue dotted line) structures at normal incidence with a LiNiO₂ thin film 354 nm thick.

FIG. 3. The absorbance as a function of frequency in $(AB)^{10}D$ (a) and (c) and $(BA)^{10}D$ (b) and (d) structures from left (right) to right (left) propagation at normal incidence with the thickness of 354 nm (a) and (b), 325 nm (c) and 236 nm (d) for $LiNiO_2$ films.

III. RESULTS AND DISCUSSIONS

$LiNiO_2$ thin films have been synthesized with different thicknesses. Using spectrophotometric analysis, the optical constants for these $LiNiO_2$ thin films have been extracted from the transmittance and reflectance spectra in the literature.²² When the wavelength is larger than $1\ \mu m$ ($1\ \mu m = 300\ THz$), the complex refractive indices (n , κ) can be treated as a constant. There are four sets of the parameters for refractive indices. (2.5, 0.24), (2.12, 0.19), (1.91, 0.13), and (1.58, 0.1) are for $LiNiO_2$ thin films of thickness 354 nm, 325 nm, 236 nm, and 200 nm, respectively. It can be seen

that the absorption increases with increasing thickness of the $LiNiO_2$ thin films. However, for a given thin film, the absorbance is finite and almost a constant at normal incidence. For example, the absorbance for the thickness of 354 nm is about 10%. When $LiNiO_2$ thin films are included as an active medium in the PC layered structure, unusual electromagnetic properties are expected. The transmittance and absorbance of $LiNiO_2$ films can be modified by the PC structures.

In the present work, the multilayer structures of $(AB)^{10}D$ and $(AB)^nD(AB)^m$ are designed. The layers A and B are dielectric materials. D indicates the $LiNiO_2$ thin film.

FIG. 4. The absorbance as a function of frequency and incident angle in $(AB)^{10}D$ and $(BA)^{10}D$ structures from left (right) to right (left) propagation with $LiNiO_2$ of 354 nm thickness for the TE mode. The color bar represents the value of absorbance.

FIG. 5. The absorbance as a function of frequency and incident angle in $(AB)^{10}D$ and $(BA)^{10}D$ structures from left (right) to right (left) propagation with $LiNiO_2$ of 354 nm thickness for the TM mode. The color bar represents the value of absorbance.

The refractive index and the thickness A (B) are taken as $n_A = 2.0$ ($n_B = 1.5$) and $d_A = 500$ nm ($n_A d_A = n_B d_B$). n and m are the layer numbers. The coated layer or the inserted layer is a $LiNiO_2$ thin film of different thickness with a different complex refractive index. $LiNiO_2$ can be treated as a defect layer inserted in the dielectric PC.

In Fig. 1, the dependence of the absorbance on frequency is shown for the structure $(AB)^n D (AB)^{10-n}$ at normal incidence with the $LiNiO_2$ thickness of 354 nm. With only one $LiNiO_2$ thin film layer, the enhanced absorption can be

modified by the dielectric PC. For different locations of the $LiNiO_2$ defect layer, the absorbance of $LiNiO_2$ thin films increases in the photonic bandgap of the (AB) PC. Another phenomenon about the dispersion relation in $(AB)^n D (AB)^{10-n}$ should be mentioned is that when the $LiNiO_2$ thin film layer is included in (AB) PC, a tunneling mode (propagation state) emerges in the photonic bandgap of the (AB) PC, which induces a strong absorption in these energy regions. Changing the width of the $LiNiO_2$ thin film, the absorption can be tuned. But the dependence of absorbance on the frequency remains

FIG. 6. The absorbance as a function of frequency and incident angle in $D(BA)^{10}$ (a) and (b) and $D(AB)^{10}$ (c) and (d) structures for the $LiNiO_2$ thickness of 236 nm (a) and (c) and 200 nm (b) and (d) for the TE mode. The color bar represents the value of absorbance.

FIG. 7. Dispersion relation between ω and the complex Bloch wavevector for $(AB)^{10}$ (a) and $(AB)^{10}D$ (b) PC at normal incidence. The thickness of $LiNiO_2$ film is 354 nm. The solid (black) and dotted (blue) lines refer to the real β' and imaginary β'' parts of the complex Bloch wavevector.

unchanged. Reducing the thickness of the $LiNiO_2$ film, the coefficient of light extinction decreases, which gives rise to weaker light absorption compared with the case for the thick $LiNiO_2$ thin film. The numerical results show that when a $LiNiO_2$ defect layer is located as far forward as possible, the absorptance can be sharply tuned by the PC. In the following, the $LiNiO_2$ thin film is placed as the first or the last layer in the multilayer dielectric structures.

In Fig. 2, the transmittance as a function of frequency for three structures, $(AB)^{10}$ PC and PC coated with a $LiNiO_2$ thin film, has been obtained. Because of the conductivity of the $LiNiO_2$ thin film, the average transmittance decreases with increasing optical frequency, together with similar oscillating structures and energy bands for (AB) PC in the transmittance spectrum. When $LiNiO_2$ thin film is included, the newly occurring propagation state in the photonic forbidden gap of (AB) PC is observed (see Fig. 7). The absorptance (reflectance) exhibits the maximum (minimum) and minimum (maximum)

value when the $LiNiO_2$ film is the first or the last layer. However the transmittance is same for the $D(AB)^{10}$ and $(BA)^{10}D$ structures.

Figure 3 shows the frequency-dependent absorptance for the layered structures $(AB)^{10}D$ and $(BA)^{10}D$. The effect of the optical transmitting direction has been investigated. The normal incident electromagnetic wave from one side to the other side shows strong absorptance, which indicates that the electromagnetic wave penetrates into the structure. However, when the light is incident from the other end, almost total reflection occurs. This one-way absorption in the photonic bandgap of (AB) PC can be used in selective-wavelength opto-electrical applications. Converting the dielectric film order from (AB) to (BA) , the absorption strength can be further adjusted as shown in Figs. 3(a) and 3(b). For the $LiNiO_2(AB)^{10}$ structure, over 95% absorption indicates that the electromagnetic wave can hardly reflect and attenuates quickly when propagating through the total system. Decreasing the thickness of $LiNiO_2$ films, the absorptance decreases as shown in Figs. 3(c) and 3(d). For all cases, a stronger absorption in the higher energy gap can be observed.

The dependence of absorptance on the frequency and the incident angle for both TE and TM modes are given in Figs. 4–6 for different $LiNiO_2$ thin film thicknesses. It can be seen that there are two one-way strong absorption regions. When the $LiNiO_2$ thin film is the first layer, the stronger absorption peak in the photonic bandgap of (AB) PC can be observed. The absorption peak shifts to higher energy as the incident angle increased which can be understood from the resonance condition $k \cos \theta \propto m$ with θ and m being the incident angle and an integer. The detailed absorption peak width and strength at different incident angles depends on the thickness of the $LiNiO_2$ thin film and the TE/TM modes. The higher energy absorption peak for $LiNiO_2(AB)^{10}$ and $LiNiO_2(BA)^{10}$ structures for the TM mode exhibits strong absorption for broader incident angles from normal incidence to grazing

FIG. 8. The photonic energy band structure for $(AB)^{10}$ PC. The dependence of the real (a) and (c) and imaginary (b) and (d) Bloch wavevectors on the incident optical energy and incident angle. (a) and (b) and (c) and (d) are for the TE and TM modes, respectively. The color bar represents the value of the real and imaginary Bloch wavevectors.

FIG. 9. Same as Fig. 8 except for $(AB)^{10}D$ PC. The thickness of $LiNiO_2$ film is 354 nm. The color bar represents the value of the real and imaginary Bloch wavevectors.

incidence. Decreasing the thickness of the thin films, the sharp and strong absorption peaks can be clearly seen for the thickness of 236 nm and 200 nm for the TE mode at large incident angles in Fig. 6.

The energy dispersion curves for the $(AB)^{10}$ and $(AB)^{10}LiNiO_2$ PC structures at normal incidence are shown in Fig. 7. There are two obvious energy gaps between 69–81 THz and 219–232 THz for $(AB)^{10}$ PC. In the presence of the $LiNiO_2$ thin film, the energy gap region broadens. But the real part of the Bloch wavevector $\beta' \Lambda$ increases from 0 to π and decreases from π to 0 in the lower and higher energy bandgaps, respectively, instead of being 0 with the imaginary part $\beta'' \Lambda$ being a finite value. These apparent tunneling

modes indicate that electromagnetic waves with frequency in the energy gap of (AB) PC can propagate but is attenuated by the propagating process which corresponds exactly to the absorption peaks in Fig. 3. From normal incidence to oblique incidence, the dependence of the complex Bloch wavevector as a function of frequency and incident angle for $(AB)^{10}$ and $(AB)^{10}LiNiO_2$ PC has been shown in Figs. 8 and 9, respectively. In a $(AB)^{10}$ PC structure, the well-defined photonic bands and bandgaps have been displayed. With $LiNiO_2$ included, because of the dielectric characteristic of the $LiNiO_2$ thin film, the phase of the interfering resonance shifts to lower frequency. And one can see that the degenerate tunneling modes within the lower energy bandgap split into

FIG. 10. The transverse electric field distribution in the structures $(AB)^{10}D$ and $D(BA)^{10}$ at the frequencies 67 THz and 217 THz in the middle of the (AB) PC gap. The light and dark gray regions indicate the dielectric A and $LiNiO_2$ film with the thickness of 354 nm.

two discrete modes at a large incident angle for the TE mode and at a small incident angle for the TM mode. These non-zero imaginary parts of the Bloch wavevector give rise to strong absorption. But when LiNiO₂ layer is coated on the top or the bottom layer, the absorptance is very different which can be understood from Fig. 10. To further illustrate the absorption property, Fig. 10 plots the distribution of the modulus of the electric field for (AB)¹⁰D and D(BA)¹⁰ structures at the frequency 67 THz and 217 THz in the middle of the two energy gaps along the propagation direction *z*. The electric field amplitude of the incident wave is supposed to be 1. As can be seen from Fig. 10, the electron motions are damped much more when LiNiO₂ film is located as the first layer. When the light beam is transmitted to the LiNiO₂ film surface, the electric field distribution at the LiNiO₂ interface in (AB)¹⁰D is much lower than in D(AB)¹⁰ which leads to different optical absorption of the LiNiO₂ film. Therefore, the strong and the weak absorptance have been observed in D(AB)¹⁰ and (BA)¹⁰D structures, respectively.

In summary, the optical transport properties of a LiNiO₂ thin film/PC hybrid structure have been analyzed theoretically and numerically. The optical propagating direction, normal incidence or oblique incidence, and TE/TM modes have been investigated. Our main findings are as follows: (i) only one layer of the LiNiO₂ thin film in the (AB) PC structures can enhance the absorption of the optical energy when the electromagnetic wave goes through the multilayer structures. (ii) The strongest and weakest absorptions can be observed in the photonic forbidden gap of the (AB) PC. (iii) The optical propagating direction can give rise to one-way absorption at the same wavelength (frequency). (iv) Decreasing the LiNiO₂ thin film thickness, the coefficient of light extinction decreases which reduces the optical absorption. (v) Tunneling modes have been obtained in the photonic energy gap of (AB) PC with the LiNiO₂ film included which leads to the modified absorption. The absorptance is dependent on the location of the defect layer. (vi) The absorption spectrum width and position can be modified effectively by the incident angle and the TE/TM modes. Our results on optical properties of (AB) PC with LiNiO₂ thin films included can be useful for developing related optoelectrical devices.

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