

# Characterization of the dynamics of photonic crystal molecules with Kerr nonlinearity by numerical pump-probe simulations

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We investigate the dynamics of photonic crystal (PC) molecules with Kerr nonlinearity by numerical simulations in a pump-probe scheme based on the finite-difference time-domain technique. The constitutional PC atoms of the nonlinear PC molecules are intentionally chosen to be multimode so that the pump and probe waves can be set at different frequencies, ensuring the clear identification of the dynamics of nonlinear PC molecules. Being more complicated than the dynamics of nonlinear PC atoms, we reveal that the coupling between the PC atoms plays an important role in determining the dynamical responses of nonlinear PC molecules to the excitation of ultrashort pulses. It is reflected in fact that PC molecules with different spectral shapes exhibit different dynamical response behaviors.

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Interest in photonic crystals (PCs) has increasingly grown in last decade due to their capability in controlling the propagation of electromagnetic waves<sup>[1,2]</sup>. So far, PCs have been widely used as a platform to manipulate the flow of light<sup>[3]</sup>. Various functional devices based on PCs have been proposed and demonstrated, such as waveguides<sup>[4,5]</sup>, power splitters<sup>[6]</sup>, wavelength demultiplexers, optical delay lines, and optical switches<sup>[7]</sup>. As compared with perfect PCs, PCs with imperfections or defects are more interesting and useful. As the simplest version of PC defects, a point defect, which is sometimes referred to as a PC atom, has been extensively studied and explored for various applications<sup>[8–10]</sup>. In particular, it can be used to build all-optical switches, a key component for ultrafast all-optical communication and optical computation in the future, when Kerr nonlinearity is introduced<sup>[11,12]</sup>. Recently, we carried out an initial study on the dynamical response of PC atoms with Kerr nonlinearity to the excitation of ultrashort pulses. Then, we proposed a numerical pump-probe simulation that can be employed to characterize the dynamics of nonlinear PC structures<sup>[13,14]</sup>.

It has been known that the coupling of two PC atoms can create a PC molecule and that of a number of PC atoms can generate a PC solid. A typical example of PC solids is coupled cavity waveguides (CCWs) that have

been considered as one of the key components for future PC integrated circuits<sup>[15,16]</sup>. The linear properties of CCWs have been extensively investigated while their nonlinear behaviors remain unexplored. As first step, we present an investigation of nonlinear PC molecules, concentrating on their dynamical response to the excitation of ultrashort pulses.

The structure of the PC molecules we studied is schematically shown in Fig. 1(a). The two-dimensional (2D) PC consists of a square lattice of dielectric rods ( $15 \times 10$ ) with a refractive index of  $n_0 = 3.4$  and a radius of  $0.2a$ , where  $a = 1 \mu\text{m}$  is the lattice constant. The constitutional PC atoms are indicated by dashed boxes. The two defects in PC molecules are introduced by modifying the radii of the central rods in the PC atoms and introducing Kerr nonlinearity into them. Thus, we have  $n(x, z) = n_0 + n_2 E^2(x, z)$  in the two defects, where  $n_2 = 0.02 \mu\text{m}^2/\text{W}$  is the nonlinear coefficient and  $E^2(x, z)$  is the local electric field intensity. A perfectly matched layer boundary condition is employed for the finite-difference time-domain (FDTD) simulation. The grid size used in the simulation is  $a/24$  for both directions. Further reduction in grid size barely influences the simulation results. The first band gap of the 2D PC for transverse magnetic polarization ranges from  $0.2824 (2\pi c/a)$  to  $0.4258 (2\pi c/a)$ .

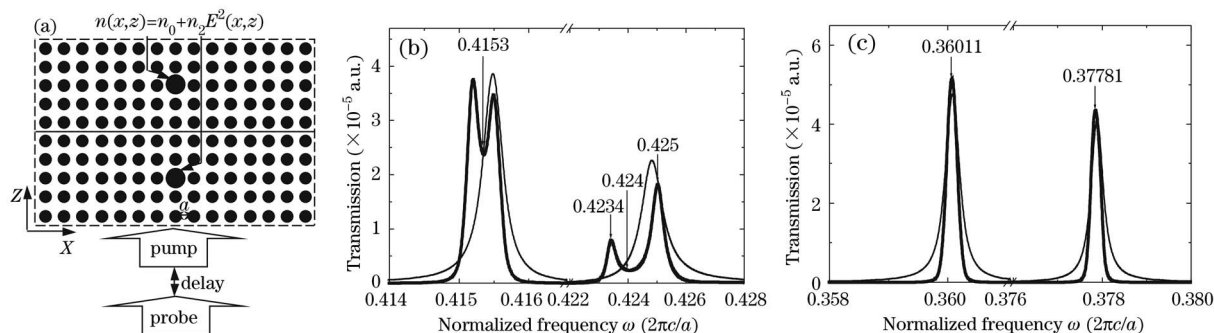


Fig. 1. (a) Structure of the 2D PC molecules. (b) Spectrum of the 2D PC molecule (thick line) in which the radius of the defects is  $0.42a$ . The spectrum of the constitutional PC atoms (thin line) is also provided for reference. (c) Spectrum of the 2D PC molecule (thick line) in which the radius of the defects is  $0.50a$ . The spectrum of the constitutional PC atoms (thin line) is also provided for reference.

In conventional pump-probe techniques, the frequencies of the pump and probe waves are generally chosen to be different in order to avoid the difficulty in detection. Thus, we choose to study PC molecules whose constitutional PC atoms are multimode. This choice makes it possible to excite the nonlinear PC molecules at one frequency while detecting their dynamical responses at another. It is well known that the spectra of PC molecules depend strongly on the coupling of the constitutional PC atoms. Therefore, we intentionally investigate two PC molecules whose spectra are completely different. The radii of the defects for the two PC molecules are chosen to be  $r_1 = 0.42a$  (molecule A) and  $r_2 = 0.50a$  (molecule B), respectively. The spectra for the two PC molecules are shown in Figs. 1(b) and (c). The spectra of the corresponding PC atoms are also provided for reference. For molecule A, the spectrum of the PC atom possesses two defect modes of Lorentz lineshapes located at  $0.4248 (c/a)$  and  $0.4155 (c/a)$ . When the two PC atoms are combined to form a PC molecule, as expected, each defect mode evolves into a structure with double peaks, corresponding to the bonding and anti-bonding states. Accordingly, the spectrum linewidth is broadened due to the coupling of PC atoms. As for molecule B, the situation is completely different. No bonding and anti-bonding states are observed in its spectrum. Instead, the spectrum appears to be similar to that of the PC atoms but with a narrower linewidth. Based on our previous studies on the coupling of PC atoms in PC molecules, the phase difference between the two PC atoms in this case happens to be  $N\pi$ , where  $N$  is an integer. In the following, it can be seen that the phase difference between the two constitutional PC atoms plays an important role in determining the dynamical response of PC molecules.

To perform the pump-probe simulations, we excite the PC molecules at the high-frequency mode and detect their dynamical response at the low-frequency one. Apparently, we have set the pump wave for molecule A. Here, we are going to examine the situations in which the pump wave are set at the bonding state ( $\omega_{\text{pump}} = 0.4234 c/a$ ), the anti-bonding state ( $\omega_{\text{pump}} = 0.425 c/a$ ) and the valley in between them ( $\omega_{\text{pump}} = 0.424 c/a$ ), as shown in Fig. 1(b). At each pump wave frequency, the dependence of the transmission spectrum on the pump power density will be evaluated. The pulse widths for the pump and probe waves are chosen to be 5 ps and 100 fs. Thus, the spectral linewidth of the pump pulse is slightly narrower than that of the excited defect mode while the spectral linewidth of the probe pulse is much broader than that of the detected defect mode. By adjusting the time delay between the pump and the probe pulses (as shown in Fig. 1), we are able to characterize the dynamics of the nonlinear PC molecules. In time domain, we intentionally make the peaks of the two pulses coincide. The peak intensity of the pump pulse appears at a time that equals twice of its width. Thus, the peak of the probe pulse appears at a time that equals 100 times of its width. As for the intensities of the two pulses, the intensity of the probe pulse is intentionally chosen to be much weaker than that of the pump pulse (i.e.,  $P_{\text{probe}} \ll P_{\text{pump}}$ ). In all simulations, the condition  $P_{\text{probe}} \leq 0.01P_{\text{pump}}$  is satisfied.

First, let us examine the evolution of the low-frequency defect mode upon the increase of pump power density

when the PC molecule is excited at the anti-bonding state. The results obtained by pump-probe simulations are presented in Fig. 2. With increasing the pump power density, the original defect mode with two peaks gradually evolves into a single-peak shape and eventually becomes a multi-peak spectrum at high excitation densities. Meanwhile, the spectrum width is significantly broadened towards low frequency and the peak transmittance is markedly reduced. As the excitation frequency is changed, even at the same pump power density, the resulting dynamical spectrum is different. In Fig. 3, we present the dynamical spectra of the low-frequency defect mode for different excitation frequencies at the same excitation density of  $0.2 \text{ W}/\mu\text{m}^2$ . It can be seen that the largest shift of the defect mode is achieved when the bonding state is excited while the smallest shift is observed when the pump wave is set at the anti-bonding state. In order to gain a deep insight into this phenomenon, we have recorded the electric field intensities in the two PC atoms for different excitation frequencies and presented them in Fig. 4. It is obvious that electric field intensities in the two PC atoms are in phase for  $\omega_{\text{pump}} = 0.4234 c/a$ . However, there exists a difference of nearly three times in peak intensity. For the other two cases, a slight difference in phase is observed for the electric field intensities in the two PC atoms and the peak intensities are almost the same. According to the physical model for the dynamical response of nonlinear PC atoms, the defect mode of a PC atom oscillates harmonically between

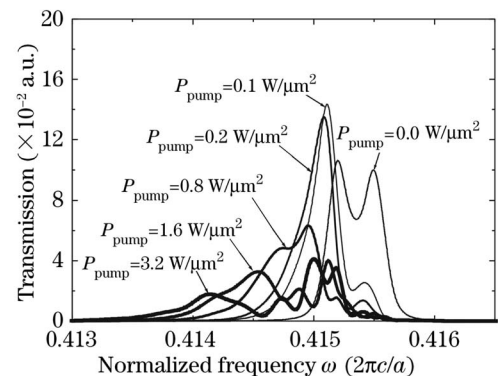


Fig. 2. Dynamical spectra of molecule A ( $r_1 = 0.42a$ ) upon the increase in pump power density at  $\omega_{\text{pump}} = 0.425 c/a$ .

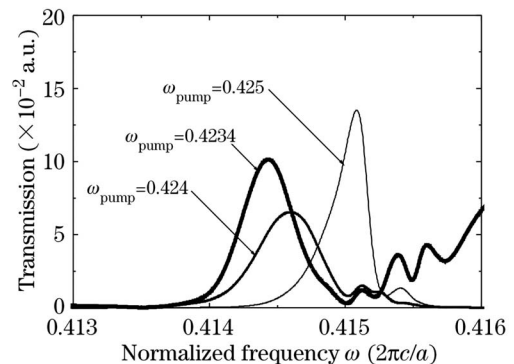


Fig. 3. Dynamical spectra of the low-frequency defect mode of molecule A for different excitation frequencies. The excitation density is  $0.2 \text{ W}/\mu\text{m}^2$ .

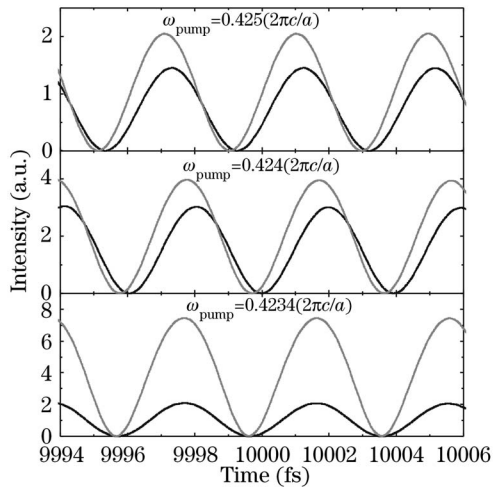


Fig. 4. Electric field intensities in the two PC atoms of molecule A for different excitation frequencies.

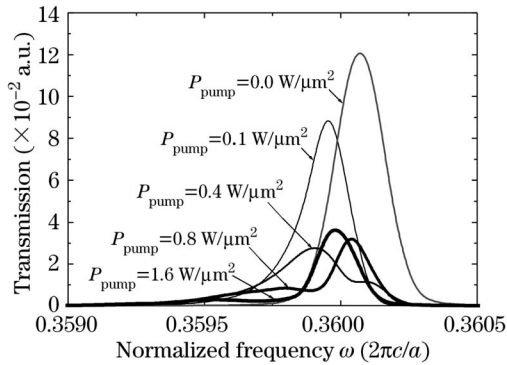


Fig. 5. Dynamical spectra of molecule B ( $r_2 = 0.50a$ ) upon the increase in pump power density.

its original position and a final position that is dependent on the electric field intensity in the PC atom. Consequently, the phase difference determines the dynamical coupling of the PC atoms. Therefore, we can conclude that the phase between the two constitutional PC atoms is crucial in determining the dynamical spectrum of the PC molecule.

Finally, let us inspect the dynamical spectrum of molecule B. The evolution of the spectrum upon the increase in pump power density obtained by numerical pump-probe simulations is shown in Fig. 5. It is apparent that the defect mode with a Lorentz lineshape shifts to low frequency with the increase of pump power density. At moderate excitation densities, another peak appears at the high-frequency side and its intensity increases gradually with increasing excitation density. At high excitation densities, only the high-frequency peak is

left and its transmittance is much lower than the original value. In summary, we have investigated the dynamics of nonlinear PC molecules by numerical simulations in a pump-probe scheme based on the FDTD technique. We intentionally choose to study PC molecules of multimode to ensure the clear identification of the dynamics. The responses of PC molecules with different spectral shapes to the excitation of ultrashort pulses are examined. It is found that the phase difference between the constitutional PC atoms plays an important role in determining the dynamical response behaviors.

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