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Journal

The Ultra-Wide Band Gap Property Induced by Lattice Period Gradually Changing in Three-Dimensional Photonic Crystals

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The lattice period gradually changing and its ultra-wide band gap property were studied in the three-dimensional diamond photonic crystals (PC) fabricated by rapid prototyping and gel casting techniques using alumina. The band gap width and center frequency of the band gap almost kept stable when the lattice period changed along the direction in vertical to the propagation direction of the electromagnetic wave. When the lattice period stretched along the propagation direction of the electromagnetic wave, the center frequency of the band gap shifted to the lower frequency range while the band gap width increased slightly. Several PCs that stretched along the electromagnetic wave propagation direction were combined together to investigate their complex band gap properties. The band gap width increased with the period change of the combined PCs. When the period change reached 134%, the band gap width became the widest and was 153% of that of the perfect PC, which agreed well with the simulation results by Ansoft HFSS.

I. Introduction

PHOTONIC crystals (PC), structures with periodic variation of dielectric constant that can manipulate the propagation of the electromagnetic wave, have attracted considerable attentions in recent years for their wide potential applications.[1–5] It is well known that three-dimensional (3D) PCs with a diamond structure can have a complete band gap.[6,7] Most of the research efforts on the diamond structure are concentrated on the fabrication method [8–12] and structures with different working frequency range.[13,14] The changes of macrostructure, such as period lattice gradually changing, are of great interest for photonic applications. However, only a few works have been focused on the study of 3D macrostructure changes. Kirihara *et al*.[15] have investigated the influences of lattice modifications along the propagation of the electromagnetic wave on the microwave emission and the band gap property.

In this work, the influence of the gradually changing of lattice period on the band gap property has been systematically studied. A perfect PC was firstly fabricated and experimentally investigated. Based on the perfect PC, a series of lattice period changed structures that stretched along the parallel and vertical directions to the propagation of the electromagnetic wave were designed and investigated. The stretched structures were combined together to investigate the changes of the band gap properties. Experimental results were compared with the simulation results obtained by Ansoft HFSS.

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II. Experimental Procedure

The rapid prototyping (RP) technique together with gel casting and sintering process were chosen as the fabrication method. First, the CAD models of the PCs with inverse diamond structure expanded from one unit cell and the CAD models of boxes to accommodate the PCs inside with the size rightly matching the PCs were made by Ansoft HFSS (V11, Ansoft Corporation, Pittsburgh, USA). The box and the PC molds were then fabricated using a RP machine (Hengtong, SPS450B, Xi'an, China). Second, the gel containing alumina was prepared to cast into the molds. The primary solution which was composed by C_3H_5NO and $C_7H_{10}N_2O_2$ mixed well with water, was prepared and the weight percentage of the organic compound is 20 wt%. The alumina powder was added into the primary solution and the dispersant $CH_2CHCOONa$ was gradually added in. The weight percentage of the alumina ceramic powder is 75 wt%. A little $NH_3 \cdot H_2O$ was dropped into the slurry to adjust the pH value to 9–10. The slurry was milled for 3 h after the activator $C_6H_{12}N_6$ was added. Then, the evocator $(NH_4)_2S_2O_8$ was added into the slurry. Third, after the diamond structure molds and the boxes were fabricated, the gel slurry was cast into the box to about a half volume. Then, putting the PC molds into the boxes and pressing the systems slightly with a pressure of 0.2 MPa, the slurry gradually permeated into the interstices of the inverse diamond structure molds. The samples were kept still for 2 h and then evacuated under −0.09 MPa to degas. The samples were dried in air at room temperature for 24 h. In the end, the samples were sintered at 1530°C for 4 h to obtain the ceramic PCs.

The lattice constant of the perfect PC was chosen as 12 mm because its band gap lies at the X-band of microwave frequency range by the simulation with Ansoft HFSS. The dimension of the perfect structure was set as 60 mm × 60 mm × 60 mm. The period lattice was then stretched 5%, 10%, 15%, 20%, and 25% based on the perfect PC along directions parallel and vertical to the propagation of the electromagnetic wave, respectively. First, the stretched molds were made by the RP technique and then the stretched PCs were obtained by the gel casting and sintering process. The stretched ratio is defined as the ratio of the stretched PC's dimension to that of the perfect PC, which means that if the period lattice is stretched 5%, the stretched ratio will be 105%. The period lattice gradually changed combined PC was made by adding the separate stretched PCs together. In order to investigate the band gap property of the period lattice gradually changed combined PC completely, several stretched PCs with stretched ratio of 130%, 134%, and 137% were also fabricated.

The PCs were measured by the transmission/reflection (T/R) methods with a waveguide cavity connecting with a network analyzer (HP 8720ES, Hewlett-Packard, Santa Rosa, CA) to obtain the propagation characteristic of the electromagnetic wave. The band diagram of the diamond PCs and the transmission property of electromagnetic wave in the PCs were simulated by Ansoft HFSS.

III. Results and Discussions

Figure 1 shows the simulation and measurement results of the perfect 3D PC. It can be observed that the band gap lies between 10.5 and 12 GHz from the simulation result. The measurement result shows a clear band gap that agreed well with that from the simulation. The real PC sample is shown in the inset with a dimension of 60 mm × 60 mm × 60 mm. It can be found that the holes and periods throughout the real PC sample keep uniformity well after sintering. The lattice constant of the structure is 12 mm and the aspect ratio (the ratio of the radius of skeleton rod, which is the diamond lattice rod, to the lattice constant) is 0.37. The fine PC indicates that the RP method together with gel casting and sintering technique is effective in the fabrication of PCs.

Figure 2 shows the relationship between the band gap properties and the stretched ratio of the PCs with the stretching direction vertical and parallel to the propagation of the electromagnetic wave. Both the center frequency of the band gap and the band gap width almost did not change when comparing with the results of the perfect PC as shown in Fig. 2(a). This result reveals that the change of the transverse structure of the PC in vertical to the propagation of the electromagnetic wave has little influence on the band gap properties of PC. According to Chern and Chao's[16] report, for the electromagnetic wave propagating in parallel to the lattice plane, the time-harmonic electromagnetic modes (with time dependence $e^{i\omega t}$) can be described as:

$$-\nabla^2 E = \varepsilon\left(\frac{\omega}{c}\right)^2 E \tag{1}$$

$$-\nabla\left(\frac{1}{\varepsilon}\nabla H\right) = \left(\frac{\omega}{c}\right)^2 H \tag{2}$$

For the periodic structures with infinite extent, it is sufficient to solve the problem in one unit cell, along with the Bloch condition

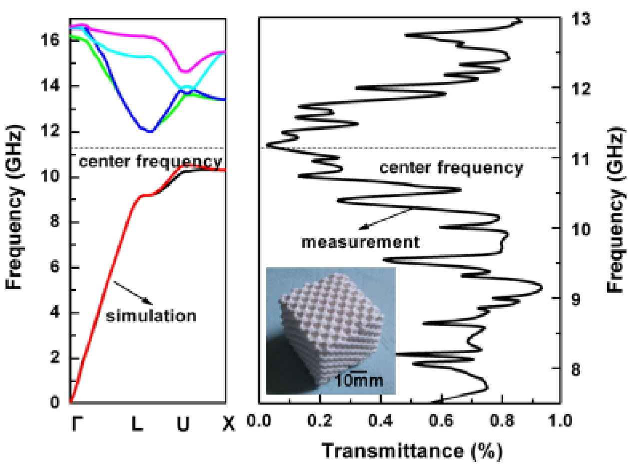

Fig. 1. The simulation and measurement results of the perfect three-dimensional photonic crystals with dimension of 60 mm × 60 mm × 60 mm.

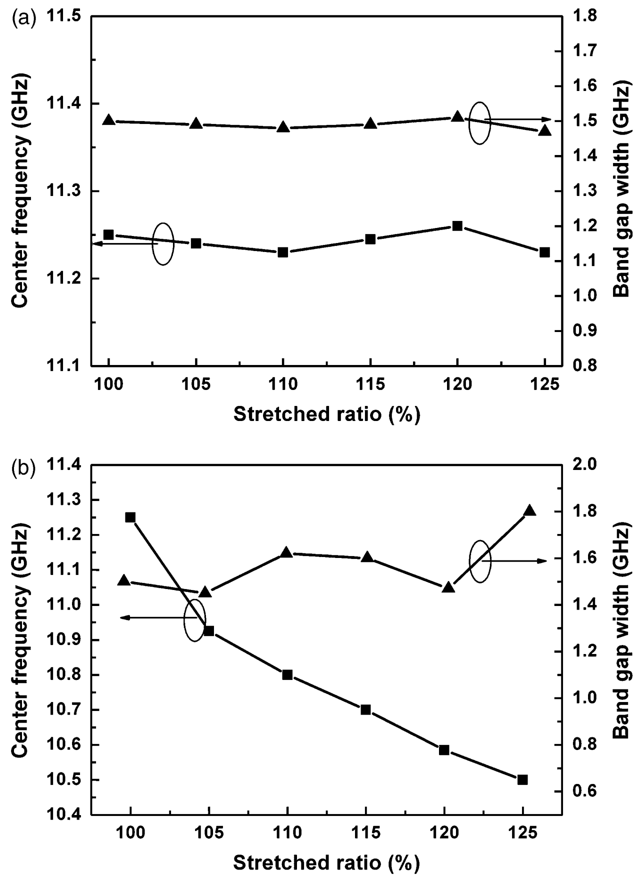

Fig. 2. The band gap properties relative with the stretching of the photonic crystals in vertical (a) and parallel (b) to the propagation of the electromagnetic wave.

$$\phi(r + a_i) = e^{ika_i}\phi(r) \tag{3}$$

applying at the unit cell boundary, where ϕ is either E or H field, K is the Bloch wave vector, and a_i ($i = 1,2$) is the lattice translation vector. Hence, if a_i does not change along the direction of r, the results of E and H field will not change according to the Bloch condition. Fig. 2(b) shows the relationship between the band gap properties and the stretched ratio along the propagation direction of the electromagnetic wave. With the increase of the stretched ratio, the center frequency of the band gap

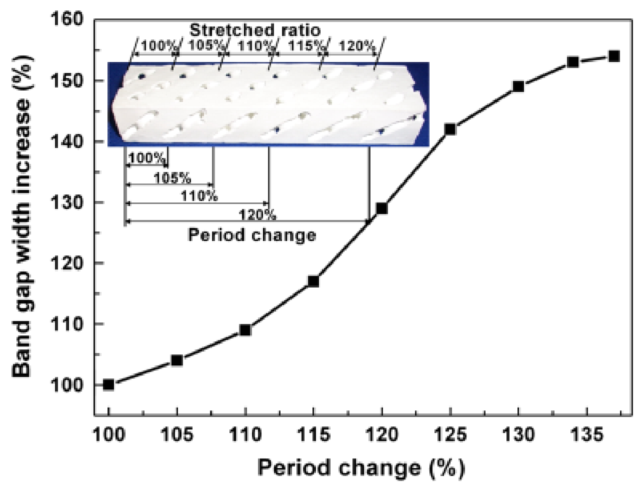

Fig. 3. The measurement result of the relationship between the band gap width and the period change of the combined photonic crystal (PC) with uniting the separate stretched PCs.

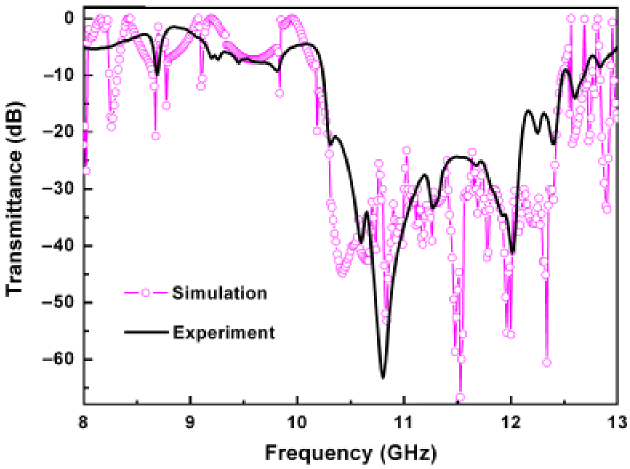

Fig. 4. The measurement (solid line) and simulation results (dash dotted line) of the combined photonic crystal with the period change 134%.

shifted toward the lower frequency and the band gap width increased slightly compared with the results of the perfect PC. When the stretched ratio reached 25%, the center frequency decreased from 11.25 to 10.5 GHz and the band gap width changed from 1.5 to 1.8 GHz. This result is in agreement with Kirihara *et al.*'s[15] report. This suggests that the lattice period changes along the direction parallel to the propagation of the electromagnetic wave can yield much influence on the band gap properties. Hence, the band gap properties can be manipulated by changing the stretched ratio along the direction in parallel to the propagation of the electromagnetic wave.

Figure 3 shows the measurement results of the relationship between the band gap width and the period change of the combined structure. The inset of Fig. 3 shows a fabricated sample that clearly expresses the stretched ratio and the period change. With the increase of the period change, the band gap width slowly increased. When the period change reached 134%, the band gap width became 153% of that of the perfect PC. If the period change continues increasing, the band gap width almost keeps the same value. This numerical value is the threshold and when the period change reaches this point the band gap width will nearly not increase. This result can be attributed to the changes of the center frequency of the stretched structures. As shown in Fig. 2(b), the center frequency of the band gap decreases with the stretched ratio along the direction in parallel to the propagation of the electromagnetic wave. The center frequency of the band gap of every separate stretched PC is different. Because the combined PC is constituted by uniting the separate stretched PCs together, the band gap width of the combined structure will increase due to the overlapping of the band gaps of every stretched PC. Furthermore, the interfaces of the separate stretched PCs are not continuous and the band gaps are formed by Bragg scattering. The discontinuous interfaces will generate interface scattering waves, which will also strengthen the Bragg scattering and increase the band gap width at last.

Figure 4 shows the measurement and simulation results of the combined PC with the period change of 134%. The measurement with a band gap from 10.2 to 12.5 GHz agreed well with the simulation result by HFSS. The band gap width is 2.3 GHz and this is 0.8 GHz wider than that of the perfect PC. Another combined PC with the period change of 137% is also fabricated and investigated and it is found that the band gap width almost does not change comparing with the period change of 134%.

IV. Conclusions

In summary, the period lattice gradually changing and its ultra-wide band gap properties were investigated by a fabrication method using RP technique together with the gel casting and sintering process. The band gap properties will not change when the PCs are stretched vertical to the propagation direction of the electromagnetic wave. When the PCs are stretched along the propagation direction of the electromagnetic wave, the center frequency of the band gap will shift to lower frequency and the band gap width will increase slightly with the increase of the stretched ratio. The band gap width of the combined PC by adding each stretched PCs together will increase with the period change. The band gap width becomes the biggest when the period change reaches 134% and the band gap width is 153% of that of the perfect PC. And the band gap width will nearly not change if the period change continues increasing.

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