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Spiral three-dimensional photonic-band-gap structure

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We found a general type of microscopic structure that can be arranged into various types of lattice to create photonic crystals with sizable band gaps. We arranged spiral-shaped rods into three types of lattice: simple cubic, face-centered cubic, and body-centered cubic; we then calculated the band structures of these dielectric structures by means of a plane-wave expansion. Our results show that there exists a gap as large as 28% for dielectric contrast of 12.25:1. [S0163-1829(98)51704-3]

The propagation of electromagnetic waves can be forbidden for all wave vectors in a certain range of frequencies in the periodic dielectric structure, which is known as photonic crystals. Owing to their ability to alter the electromagnetic radiation field and control the spontaneous emission, these photonic crystals have promising applications in optoelectronic devices, such as very high-efficiency single mode light-emitting diodes and zero-threshold semiconductor lasers.[1]

A large photonic band gap arises when the microscopic Mie resonance occurs at the same frequency as the macroscopic Bragg resonance. Thus, the existence of photonic band gaps can be interpreted as a direct result of the coalescence of Mie scattering resonances of the individual scatterers.[2] Theoretical studies have been conducted to investigate through various types of lattice structure.[3] These studies seem first to focus on the macroscopic spatial arrangement of the scatterers, i.e., the type of lattice, whether it is simple cubic (sc), face-centered cubic (fcc), or body-centered cubic (bcc), and then second to find the local structure that helps breaking symmetries and forms the band gaps specifically for those types of lattice. To our knowledge, there has been no report about a general local structure that can be applied to any type of lattice to create photonic crystals.

In this work, we show that there exists a general local geometry that breaks symmetries and forms the photonic band gaps regardless of its macroscopic lattice. We found local structures of spiral rods that can be arranged in sc, fcc, or bcc lattices to create photonic crystals with sizable band gaps.

Our idea of a spiral-shaped local element emerged from the following consideration. By connecting the lattice points of a structure known to possess photonic band gaps like diamond structure,[4] stacked-bar structure,[5] or Yablonovitch-Gmitter-Leung (YGL) structure,[6] one can find a spiral. For instance, a spiral line is found along the (001) axis from point (1/2,1/2,0)→(1/4,1/4,1/4)→(1/2,0,1/2)→(3/4,1/4,3/4)→(1/2,1/2,1) as depicted in Fig. 1. A spiral line in YGL structure can be found from point (0,0,0)→(1/2,0,1/2)→(1,1/2,1/2)→(1,1,1) along the (111) axis. Thus, we can imagine a local element being spiral shaped and these spiral-shaped rods can be arranged in sc, fcc, or bcc lattices to form photonic band gaps. This corresponds to placing an infinitely long spiral rod into a square lattice for the sc case, and, furthermore, the adjacent spiral rods are mutually half period shifted for the fcc and bcc cases.

We have calculated the photonic band structures in three lattice types: sc, fcc, and bcc. We used the standard plane-wave expansion method with about 750 planes waves. The spiral structures were represented in a fine grid of $64\times 64\times 64$ points and numerically Fourier transformed by fast

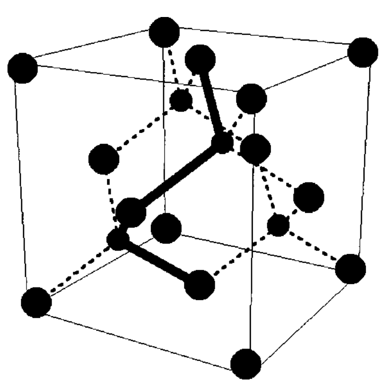

FIG. 1. A spiral that can be seen in diamond structure.

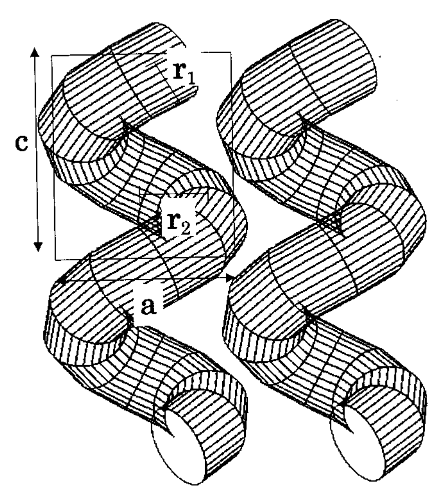

FIG. 2. Spiral structure.

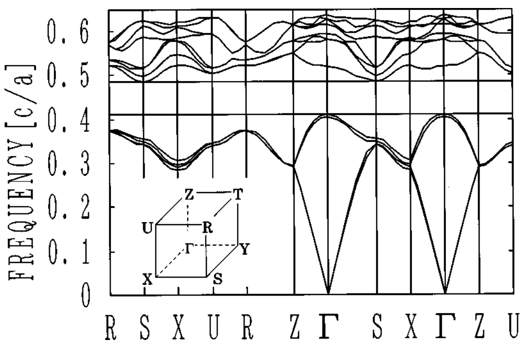

FIG. 3. Photonic band structure for the sc structure. $\varepsilon_a=1$, $\varepsilon_b=12.25$, $r_1=0.34a$, $r_2=0.34a$, $f=79\%$, and $\Delta\omega/\omega_g=16.8\%$.

Fourier transform. The dielectric constant ratio is fixed to 12.25:1 for all cases. The spiral rods with a circular cross section are shown in Fig. 2. We define r_1 as the radius of the cross section of the spiral and r_2 as the radius of the spiral itself. In Fig. 3 we show the photonic band structure of the sc structure. The band gap is found between the fourth and the fifth band for the sc lattice.

For a dielectric background, a band gap (measured by gap to midgap ratio $\Delta\omega/\omega_g$) of 16.8% is obtained when $r_1=r_2=0.34a$ (where a is the lattice constant) and the *air* fill fraction f is about 79%. From our experiences, the preferable air fill fraction for this dielectric constant ratio lies between 70% and 90%. In an air background case, if we allow spiral rods to stretch out in z axis, a small gap of about 3% appears when the z axis constant becomes $1.35a$ and $r_1=0.13a$, $r_2=0.66a$, and $f=17\%$ and $f=83\%$.

For the fcc lattice, as shown in Fig. 4, the gap lies between the second and the third band. For a dielectric background, we found a band gap of 19.5% when $r_1=r_2=0.25a$ and $f=77\%$. The structure of this case can be considered a kind of diamondlike structure and it should be since it is a diamond structure that these spiral rods are derived from. For an air background, we found an interesting case where the adjacent spiral rods do not overlap or even touch each other. The gap arises for 17.2% when $r_1=0.08a$, $r_2=0.16a$, and $f=89\%$. A larger gap of 27.8% can be obtained with $r_1=0.11a$, $r_2=0.16a$, and $f=79\%$ where the adjacent rods overlap each other.

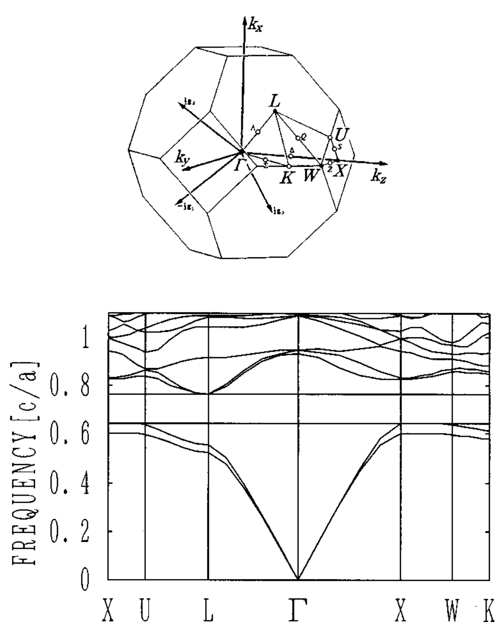

FIG. 4. Photonic band structure for the fcc structure. $\varepsilon_a=12.25$, $\varepsilon_b=1$, $r_1=0.08a$, $r_2=0.16a$, $f=89\%$, and $\Delta\omega/\omega_g=17.2\%$.

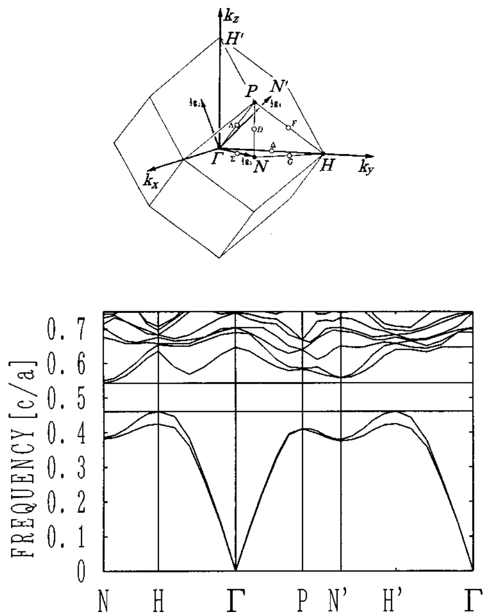

FIG. 5. Photonic band structure for the bcc structure. $\varepsilon_a=12.25$, $\varepsilon_b=1$, $r_1=0.13a$, $r_2=0.22a$, $f=82\%$, and $\Delta\omega/\omega_g=16.7\%$.

In Fig. 5, we show the band structure for the bcc lattice. For a dielectric background, there exists a 20.0% gap when $r_1=r_2=0.35a$ and $f=86\%$. This structure can be considered the same as the fcc case except that the [001] axis lattice constant is compressed to $1/\sqrt{2}$ time of itself; the result is that the gap arises a bit from 19.5% to 20.0%. Similarly for the air background case, the structure with $r_1=0.13a$, $r_2=0.22a$, and $f=82\%$ possesses a 16.7% band gap.

We have seen from the calculation that the spiral structure is favored for the photonic band gaps in various kinds of lattice. That is, there exists a general type of microscopic structure that can be applied to various kinds of lattice to create photonic band gaps. This fact also suggests that the crucial factor in the formation of photonic band gaps is the microscopic structure rather than the macroscopic one in the general case, i.e., it is the local structure of ''atoms'' in the lattice that is the determining factor in the formation of gaps, not the type of lattice. The supporting observation was reported recently in Ref. 7 for the two-dimensional (2D) case. Here, we showed the evidence in the 3D case.

In conclusion, we have shown that the spiral elements, as observed in diamond structure, possess photonic band gaps in at least three types of lattice: sc, fcc, and bcc. This means that there exists a general local geometry that breaks symmetries and forms the photonic band gaps regardless of its macroscopic lattice. Therefore, we expect to find more examples of the local structure exhibiting similar characteristics since this spiral structure and its emerging partners can provide a new approach for understanding the underlying topological physics of photonic crystals.

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