Multiphysics software gazes into photonic crystals

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Using simulation software such as COMSOL Multiphysics it is possible to calculate the band-structure diagrams of photonic crystals. This article reviews steps in the modeling process and shows how the results can evaluate potential applications.

Photonic crystals

Photonic crystals, (PhCs), [1,2], are build up by a spatial modulated index of refraction. Photons, travelling through such systems, will see a periodic change of a "potential", like electrons would encounter a periodic change of the electric potential in an atomic crystal. The first step to simulate such a system is to reduce the numerical effort. It is sufficient to calculate just the unit cell (**Fig. 1**). The material function is given by the permittivity $\varepsilon(\boldsymbol{r} + \boldsymbol{R}) = \varepsilon(\boldsymbol{r})$ and the translation vector **R**.

The underlying equations that must be solved are the Maxwell relations. PhCs are scalable, that is, numbers are assigned to the lattice constant in normalized form. For the 2D hexagonal lattice the lengths in the high symmetry directions are $|\boldsymbol{K}| = 2\pi\,(2/3)$ and $|\boldsymbol{M}| = 2\pi\sqrt{1/3}$, with these lengths enclosing an angle of 30°.

The notation for describing the polarization in PhCs differs from that used in COMSOL. To prevent any confusion, note that:

- TM = E_z polarization corresponds to TE in COMSOL
- TE = H_z polarization corresponds to TM in COMSOL

Band-structure calculations using FEM

The Maxwell equations could be reduced to two possible presentations (E and H) of the wave equation. The H presentation is preferred because it is Hermitian for real permittivities and always yields real eigenfrequencies for positive dielectric numbers:

$$\nabla \times \left(\frac{1}{\varepsilon(\boldsymbol{r})} \nabla \times \boldsymbol{H}\right) = \omega^2 \boldsymbol{H} \qquad (1)$$

For lattice-periodic systems, the Bloch function Ansatz is convenient:

$$\boldsymbol{H}(\boldsymbol{r}+\boldsymbol{R}) = \boldsymbol{u}(\boldsymbol{r}+\boldsymbol{R}) e^{ik_{\mathrm{Bloch}}(r+R)} = \boldsymbol{u}(\boldsymbol{r}) e^{ik_{\mathrm{Bloch}} r} e^{ik_{\mathrm{Bloch}} R} \qquad (2)$$

Here $\boldsymbol{R}$ is any translation vector of the lattice. In other words, the neighbouring cell of the unit cell possesses the same Bloch function except that it is corrected by the phase factor $e^{ik_{\mathrm{Bloch}}R}$. If the Bloch approach is applied in Eq. 1, it follows that

$$(i\boldsymbol{k} + \nabla) \times \left(\frac{1}{\varepsilon(\boldsymbol{r})} (i\boldsymbol{k} + \nabla) \times \boldsymbol{u}\right) = \omega^2 \boldsymbol{u} \qquad (3)$$

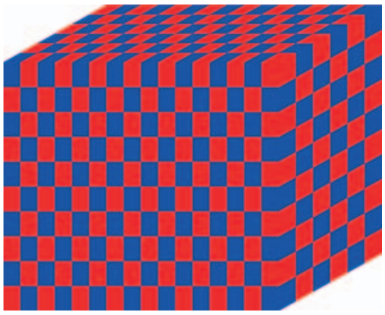

Fig. 1 3D crystal consisting of two components in a cubic system.

Choosing a Bloch vector, $\boldsymbol{k}$, that lies within the Brillouin zone and solving Eq. 3 yields the accompanying eigenfrequencies.

In order to determine eigenfrequencies of the PhC with the FEM solver, the periodicity must be established. To this end, the 2D eigenvalue solver in the RF Module of COMSOL is used. In the presentation selected, the Cartesian x-direction corresponds to the ΓK direction, and the bisecting direction to the ΓM direction. In the following, only eigenfrequencies are calculated for the TM = E_z polarization. The constraints for this are perfectly magnetic. Then the link of the boundary fields is selected with the option of the periodic constraints:

$$E_{\mathrm{left}} = E_{\mathrm{right}}\, e^{-ik_x}$$

$$E_{\mathrm{bottom}} = E_{\mathrm{top}}\, e^{-i\sqrt{3}/2 k_y - i k_x 0,5}$$

$$k_{\mathrm{Bloch}} = (k_x, k_y)^{\mathrm{T}}$$

where k_x and k_y are constants.

If a Bloch vector is now selected and the problem has been solved, eigenfrequencies for this vector are obtained. **Fig. 2** shows the field distribution belonging to the second eigenfrequency. COMSOL yields

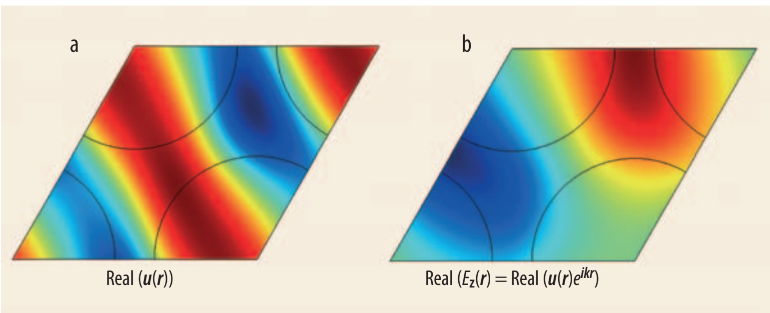

Fig. 2 Bloch (a) and crystal function (b) of the second band of the hexagonal crystal with air holes $r/a = 0.385$ in silicon $\varepsilon = 11.6$ at the ΓK point. The Cartesian x-direction corresponds to the ΓK direction. The opening angle of the rhombus is 60° and the length of a side is 1.

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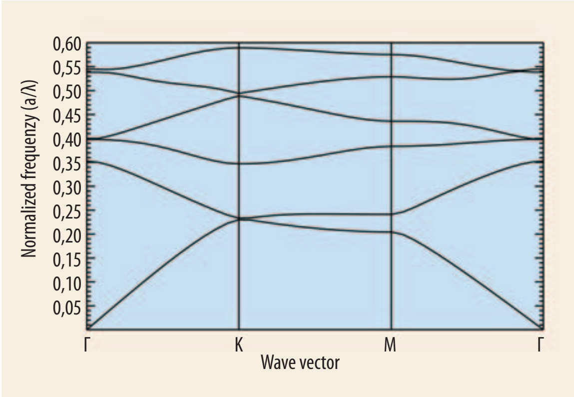

Fig. 3 Band structure of a hexagonal crystal as described in Fig. 2 (E_z polarization).

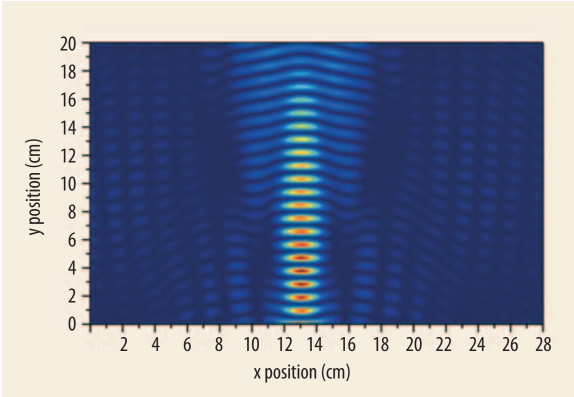

Fig. 4 Calculated beam focusing through a PhC $|\mathrm{Real}(E_z)|^2$ calculation at 18 GHz. The air holes have $r/a = 0.4$ in PMMA with $\varepsilon = 2.6$.

the function $E_z = \boldsymbol{u}(\boldsymbol{r})e^{ik_{\mathrm{Bloch}}r}$ directly. In order to obtain the Bloch function, it is still necessary to divide by the exponential function. Unfortunately, it is not possible to calculate a band structure with the aid of the software's user interface; to do so would require a parametric eigenvalue solver that varies the Bloch vector and notices all eigenvalues. A workaround is offered by COMSOL Script or MATLAB. The results of a band structure calculation of this type appear in **Fig. 3**.

Applications

PhCs offer some interesting potential applications:

Negative refractive index effect: Much has already been written about the negative refractive index [3–6]. Simulations show that this effect can also be generated with a low-refractive material such as the plastic PMMA in the microwave range $\varepsilon = 2.6$ (10–20 GHz). **Fig. 4** shows a calculation at 18 GHz with air holes of $r = 10$ mm in a hexagonal arrangement in PMMA. An X-band adapter serves as the source. Experimental results match this prediction well.

Microwave resonators: Resonators can also be produced with PhCs. The one discussed here is a hexagonal crystal composed of metal rods ($r/a = 0.2$). To calculate the band structure, the edges of the rods must be set to perfect electrical conductors. In order to obtain resonator properties, a defect must be included in the crystal. A quadrupole defect arrangement fulfils this task. Four of the nearest neighbour rods are removed for this defect (two in the Γ**K** and two in the Γ**M** direction). A quadrupole resonator of this type has been constructed. **Fig. 5** shows a 3D calculation that also sketches the structure. The lattice spacing is approximately $a = 6$ mm, and the resonance frequency is $f_0 = 18$ GHz.

The predicted resonance was found during one measurement. Its quality, Q, indicates how well a resonator can store energy:

$$Q = \text{Energy in the resonator}/\text{Energy loss after one period} \approx 2\pi \cdot f_0/\Delta f_{1/2}$$

where f_0 is the central frequency and $\Delta f_{1/2}$ the breadth of the resonance at which the intensity drops to half the value. In this case Q is approximately 4600.

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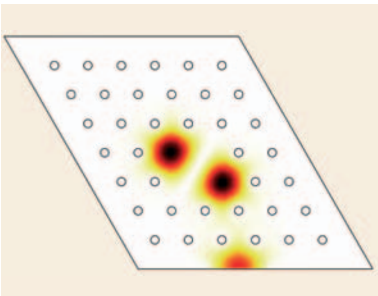

Fig. 5 Resonator structure with electrical energy density color-coded. The lattice constant is approximately $a = 6$mm. Energy is added from below through a microwave port.

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