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Modelling and design of complete photonic band gaps in two-dimensional photonic crystals

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Abstract. In this paper, we investigate the existence and variation of complete photonic band gap size with the introduction of asymmetry in the constituent dielectric rods with honeycomb lattices in two-dimensional photonic crystals (PhC) using the plane-wave expansion (PWE) method. Two examples, one consisting of elliptical rods and the other comprising of rectangular rods in honeycomb lattices are considered with a view to estimate the design parameters for maximizing the complete photonic band gap. Further, it has been shown that complete photonic band gap size changes with the variation in the orientation angle of the constituent dielectric rods.

Keywords. Photonic crystal; complete photonic band gap; plane-wave expansion method.

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1. Introduction

Photonic band gap structures/photonic crystals, especially two-dimensional (2D) photonic crystals, which are dielectric structures periodic on length scale, have recently achieved much attention, as they are easier to fabricate than 3D photonic crystals and are expected to have wide application in the design and development of ultra-small-scale optical devices. The propagation of radiation in such structures can be described similar to the case of electrons propagating in a crystal. One of the reasons for the intense investigations, both theoretical and experimental, lies in the possibility of the substantial control of the radiation field by means of these structures. These structures can exhibit a forbidden band of frequencies, or a band gap in their electromagnetic dispersion relations (ω vs. k), if the geometrical structures and the dielectric constant of the photonic lattices are appropriately chosen. The search for the structures that possess wide photonic band gap (PBG) in the frequency range of interest for various applications has motivated a lot of research. To prevent the propagation of the waves, whatever its direction is, the gaps that open at different points of the Brillouin zone must overlap as much as possible so as to give large complete band gaps. Thus it is desirable, that the different band gaps are large and centered on neighboring frequencies. However, the complete photonic band gap can be obtained in the photonic crystals in few select structures.

Several studies have been done to study the modifications in photonic band gaps in various designs of photonic crystals. The existence of complete photonic band gap allows strong photon localization within the gap and a detailed manipulation of photonic defect states. They have important applications in defect cavities, optical waveguides, defect mode photonic crystal lasers, and feedback mirror in laser diodes. Two-dimensional photonic band gap consisting of lattices with different symmetries and scatterers of various shapes, orientations and sizes have been studied numerically [1,2]. It has been shown that the periodic arrays of low index rods with either a square or a circular cross-section located on a square lattice in a dielectric background of higher index exhibit photonic band gaps common to s and p polarizations. Also two-dimensional square and hexagonal lattices of air holes in high dielectric medium generate band gaps common to s and p polarizations forming complete photonic band gap [3,4]. A large complete or absolute photonic band gap can be obtained in 2D square and triangular lattice of cylinders by introducing anisotropy in material dielectricity [5]. It can also be obtained in 2D triangular lattice of air holes with varying roundedness in dielectric and in 2D rectangular lattice of elliptical air holes in dielectric [6–8]. However, most of the studies on the existence of complete photonic band gap have been done on the 2D photonic crystals composed of air holes in dielectric media. The complete photonic band gap can be obtained in the photonic crystal composed of dielectric rods in air. As an empirical rule of thumb, transverse magnetic (TM) band gaps are favored in a lattice of isolated high dielectric regions and transverse electric (TE) band gaps are favored in a connected lattice [9]. This paper deals with partial or pseudophotonic band gaps. Further, photonic band gaps for TE and TM modes occur at different frequency regions and only in select structures both of them exist at the same frequency region giving rise to complete photonic band gap. In this paper we first investigate the existence of complete photonic band gap in photonic crystal structures and, to obtain a complete photonic band gap isolated spots as well as connected regions of dielectric material are required. Such a requirement can be fulfilled by photonic crystal composed of honeycomb lattice of dielectric rods in air. We then study the variation of complete photonic band gap size with the change in shape and orientation of constituent dielectric rods with a view to estimate the size of the complete photonic band gap for given designs of 2D photonic crystals, which can prove helpful in the design of various photonic devices operational in the range of complete photonic band gap [10,11]. Very recently, a large number of photonic devices like couplers, switches and polarization splitters have been reported involving polarization-dependent photonic band gap materials [12–14], in which knowledge of engineering photonic band gap is essential.

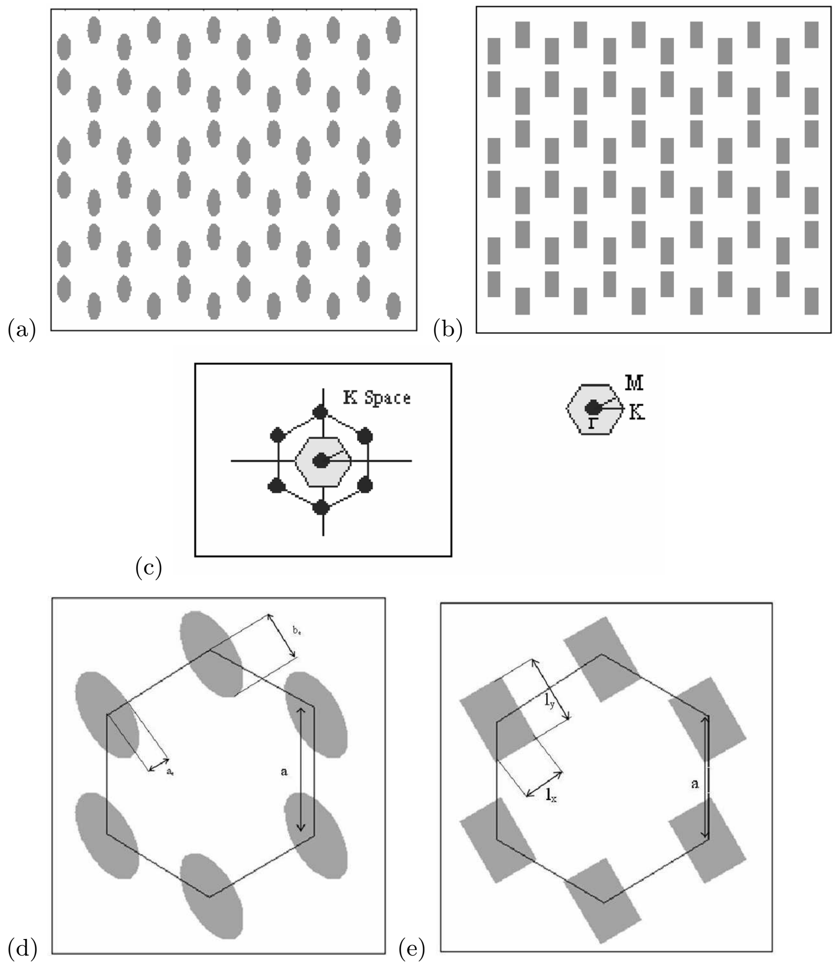

Figure 1. (**a**) PhC consisting of honeycomb lattice of elliptical GaAs rods in air. (**b**) PhC consisting of honeycomb lattice of rectangular GaAs rods in air. (**c**) Brillouin zone of the honeycomb lattice of elliptical/rectangular rods in air (inset of the figure shows the symmetry points). (**d**) Model of PhC composed of elliptical GaAs rods in air in honeycomb lattice. (**e**) Model of PhC composed of rectangular GaAs rods in air in honeycomb lattice.

2. Design parameters

To analyse the variation of complete photonic band gap size in 2D photonic crystals, we consider the following two structures of photonic crystals: (1) Elliptical GaAs rods ($n = 3.376$) in air in honeycomb lattice as shown in figure 1a, (2) rectangular GaAs rods ($n = 3.376$) in air in honeycomb lattice as shown in figure 1b.

Figure 1c shows the Brilllouin zone for the two structures used to study the variation of complete photonic band gap size. Figure 1d depicts the model of the

PhC consisting of elliptical rods in air in honeycomb lattices where a is the lattice constant, a_{e} and b_{e} are the minor and major radii of the constituent elliptical rods respectively. Figure 1e shows the model of the PhC consisting of rectangular rods in air in honeycomb lattice where a is the lattice constant, l_x and l_y are the sides of the constituent rectangular rods such that $l_x \leq l_y$ respectively.

The materials used to study the effect of ellipticity on the photonic band gaps consist of GaAs and air as they provide adequate dielectric contrast for obtaining photonic band gaps. Moreover, GaAs is one of the most commonly used materials in the design of various devices.

3. Numerical analysis and results

In order to calculate the band structure of the photonic crystals theoretically, the plane-wave expansion (PWE) method was employed, where both the electromagnetic field and periodic dielectric structure are expanded in a Fourier series. For that we assume the material to be linear, locally isotropic and periodic with lattice vectors $\mathbf{R}$. The relative permeability μ is taken as 1 and the relative permittivity is defined as

$$\varepsilon(\mathbf{r}) = \varepsilon_{\mathrm{b}} + (\varepsilon_{\mathrm{s}} - \varepsilon_{\mathrm{b}}) f(\mathbf{r}), \tag{1}$$

($f(\mathbf{r})$ equals 1 inside the column and 0 outside it) where ε_{s} is the dielectric constant of the columns and ε_{b} is the dielectric constant of the background.

Because of the two-dimensional lattice periodicity, the dielectric constant ε can be described by

$$\varepsilon(\mathbf{r}) = \varepsilon(\mathbf{r} + \mathbf{R}), \tag{2}$$

where vectors $\mathbf{R}$ are the vectors of the 2D lattice.

Solving Maxwell's equations for the magnetic field $\mathbf{H}_\omega$ leads to the following vector wave equation:

$$\nabla \times \left(\frac{1}{\varepsilon(\mathbf{r})} \nabla \times \mathbf{H}_\omega(\mathbf{r}) \right) = \left(\frac{\omega}{c} \right)^2 \mathbf{H}_\omega(\mathbf{r}). \tag{3}$$

The magnetic field $\mathbf{H}_\omega$ is then expanded into plane waves of wave vector $\mathbf{k}$ with respect to the 2D reciprocal lattice vectors $\mathbf{G}$

$$\mathbf{H}_\omega(\mathbf{r}) = \sum_{\mathbf{G}\lambda} h_{\mathbf{G}\lambda} \hat{\mathbf{e}}_\lambda \mathrm{e}^{[i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}]}, \tag{4}$$

where the polarization vectors $\hat{\mathbf{e}}_\lambda$ characterize two independent polarizations λ.

Substituting eq. (4) in the vector wave eq. (3) provides an equation for the coefficients $h_{\mathbf{G}\lambda}$ given by

$$\sum_{\mathbf{G}'\lambda'} \mathbf{E}^{\mathbf{k}}_{\mathbf{G}\lambda,\mathbf{G}'\lambda'} h_{\mathbf{G}'\lambda'} = \omega^2 h_{\mathbf{G}\lambda}. \tag{5}$$

The matrix $\mathbf{E}$ in the eigenvalue equation is defined by

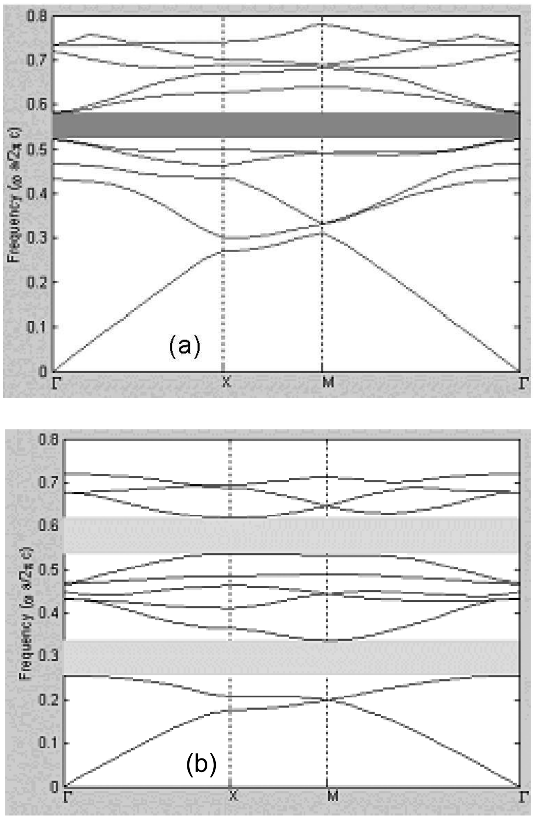

Figure 2. (**a**) Band diagram for the 2D photonic crystal composed of circular dielectric rods in honeycomb lattice with $r/a = 0.24$ in air for TE polarization. (**b**) Band diagram for the 2D photonic crystal composed of circular dielectric rods in honeycomb lattice with $r/a = 0.24$ in air for TM polarization.

$$\mathbf{E}^{\mathbf{k}}_{\mathbf{G}\lambda,\mathbf{G}'\lambda'} = [(\mathbf{k}+\mathbf{G})\times\hat{\mathbf{e}}_{\lambda}][(\mathbf{k}+\mathbf{G}')\times\hat{\mathbf{e}}_{\lambda'}]\varepsilon^{-1}(\mathbf{G},\mathbf{G}'). \tag{6}$$

The Fourier transform of the inverse dielectric constant

$$\varepsilon^{-1}(\mathbf{G},\mathbf{G}') = \varepsilon^{-1}(\mathbf{G}-\mathbf{G}') \tag{7}$$

depends on the difference of the reciprocal lattice vectors only. The properties of $\varepsilon(\mathbf{r})$ are given by

$$\varepsilon^{-1}(\mathbf{G}) = \frac{1}{A}\int_{A}\varepsilon^{-1}(\mathbf{r})\mathrm{e}^{-i\mathbf{G}\mathbf{r}}\mathrm{d}^{2}\mathbf{r}, \tag{8}$$

where A is the area of the unit cell.

By solving eq. (6) for 2D photonic crystals and in plane propagation, the photonic band diagrams are obtained for both TM and TE polarizations.

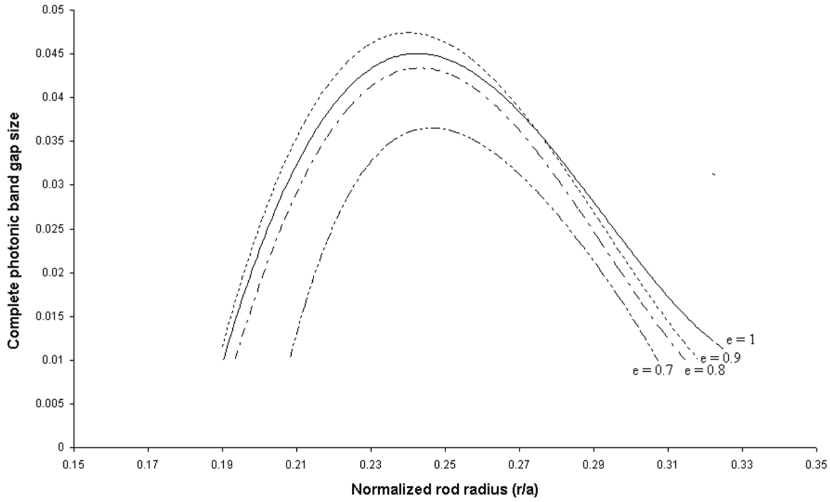

Figure 3. Variation of complete photonic band gap size with normalized rod radius (r/a) for a PhC composed of honeycomb lattice of elliptical GaAs rods ($n = 3.376$) in air for $e = 1$, 0.9, 0.8 and 0.7 keeping fill factor constant.

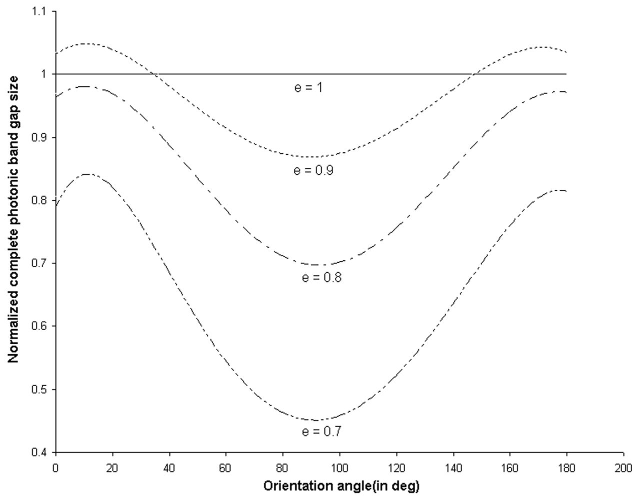

Figure 4. Variation of complete photonic band gap size with the orientation angle of constituent elliptical GaAs rods ($n = 3.376$) with $r/a = 0.24$ in air in honeycomb lattice for $e = 1$, 0.9, 0.8 and 0.7.

3.1 *Honeycomb lattice of elliptical dielectric rods in air*

We first consider the photonic crystal composed of elliptical dielectric rods in air in honeycomb lattice. The variation of photonic band gaps in the case of elliptical rods/rectangular rods has been studied under the following headings.

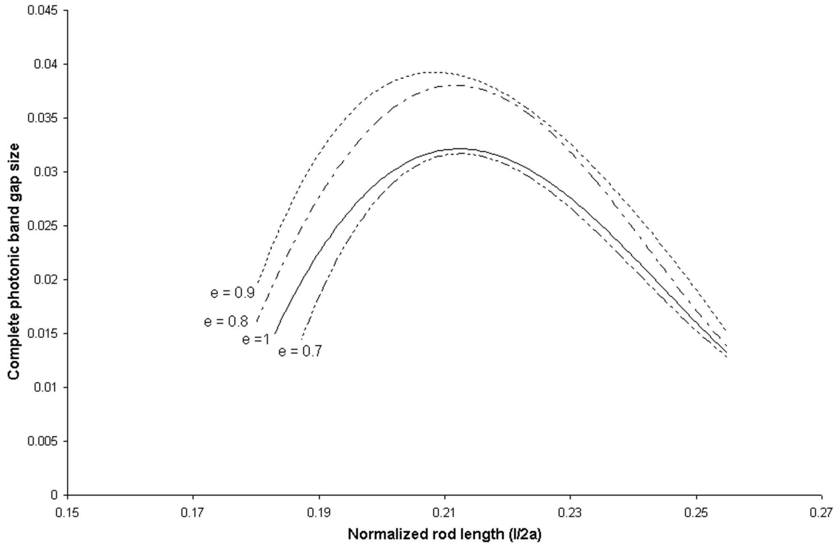

Figure 5. Variation of complete photonic band gap size with normalized rod length ($l/2a$) for a PhC composed of honeycomb lattice of rectangular GaAs rods ($n = 3.376$) in air for $e = 1$, 0.9, 0.8 and 0.7 keeping fill factor constant.

1. Keeping fill factor ($\pi ab = l_x l_y =$ constant)
2. Changing the orientation angle of the constituent dielectric rods.

The complete photonic band gap (CPBG) in the two structures results from the overlap of TE5-6 band gap (i.e. the gap between the fifth and sixth photonic bands for TE mode) and TM7-8 photonic band gap (i.e. the gap between the seventh and eighth photonic bands for TM mode) as shown in the band diagrams in figures 2a and 2b.

Figure 3 shows the variation of complete band gap size with the normalized rod radius (r/a) for four different ellipticities, namely, $e = a_{\mathrm{e}}/b_{\mathrm{e}} = 1$, 0.9, 0.8 and 0.7 keeping fill factor constant. Here, the complete photonic band gap size is defined as the direct difference between the maximum and minimum values of the complete photonic band gap limit.

We then investigate the variation in the complete photonic band gap size with the change in the orientation angle of the constituent GaAs rods. Figure 4 shows the variation of the normalized complete photonic band gap size for $r/a = 0.24$, where the maximum complete photonic band gap is obtained for $e = 1$, with the change in the orientation angle of the constituent elliptical rods for all the four cases, i.e. $e = 1$, 0.9, 0.8 and 0.7. Here the complete photonic band gap size has been normalized with the complete photonic band gap size for $e = 1$.

3.2 *Honeycomb lattice of rectangular GaAs rods in air*

We perform similar analysis for the photonic crystal composed of honeycomb lattice of rectangular GaAs rods in air. Figure 5 shows the complete band gap size variation

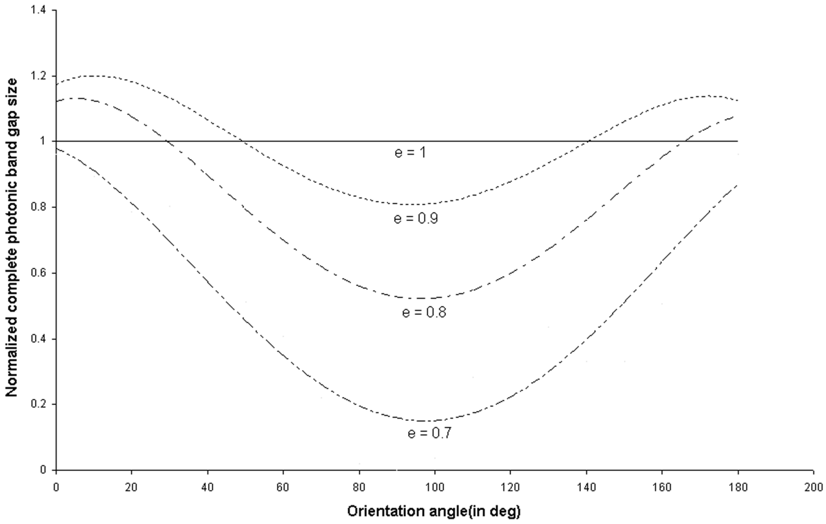

Figure 6. Variation of complete photonic band gap size with the orientation angle of constituent rectangular GaAs rods ($n = 3.376$) with $l/2a = 0.21$ in air in honeycomb lattice for $e = 1$, 0.9, 0.8 and 0.7.

with the normalized rod length (l/a) for four different aspect ratios ($e = l_x/l_y$), namely, $e = 1$, 0.9, 0.8 and 0.7.

Figure 6 shows the variation of the normalized complete band gap size for $l/2a = 0.21$ with the change in the orientation angle of the constituent rectangular rods for all the four cases, i.e., $e = 1$, 0.9, 0.8 and 0.7.

4. Discussion and conclusion

Figures 3 and 5 show that the complete band gap size first increases with the increase in fill factor and then starts decreasing with the increase in fill factor. The graphs indicate that the slight introduction of asymmetry increases the size of complete band gap. But as the constituent rods become more elliptical or rectangular in the respective cases, the size of the complete photonic band gap is reduced as compared to the case of PhC composed of circular or square dielectric rods. Figures 4 and 6 show the variation of the complete photonic band gap size with the change in the orientation angles and it is observed that after 180° rotation the structure provides the same complete photonic band gap as we started with. This can be explained on the basis of symmetry considerations.

In conclusion, we have presented the variation of complete photonic band gap size with the introduction of asymmetry in 2D photonic crystals composed of dielectric rods in air in honeycomb lattices. The study can prove useful in the design of various complete photonic band gap-based devices, where it will be important to find or engineer structures with correct band structure characteristics and hence in the design of compact all integrated photonic circuits.

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References

[1] R Wang and X H Wang, *J. Appl. Phys.* **90**, 4307 (2001)
[2] D Cassagne, C Jouanin and D Bertho, *Phys. Rev.* **B53**, 7134 (1996)
[3] P R Villeneuve and M Piche, *Phys. Rev.* **B46**, 4969 (1992)
[4] P R Villeneuve and M Piche, *Phys. Rev.* **B46**, 4973 (1992)
[5] Z Y Li, B Y Gu and G Z Yang, *Phys. Rev. Lett.* **81**, 2574 (1998)
[6] R Hillerbrand and W Hergret, *Solid State Commun.* **115**, 227 (2000)
[7] R Hillerbrand, W Hergret and W Harms, *Materials Science in Semiconductor Processing* **3**, 493 (2000)
[8] M Qiu and S He, *Phys. Rev.* **B60**, 10610 (1999)
[9] Y Kalra and R K Sinha, *Pramana – J. Phys.* **67**, 1155 (2006)
[10] L Wu, M Mazilu, J-F Gallet, T F Krauss, A Jugessur and R M De La Rue, *Opt. Lett.* **29**, 1620 (2004)
[11] R K Sinha and Y Nagpal, Paper presented at the *Seventh International Conference on Optoelectronics, Fiber Optics and Photonics*, Cochin, India, 9–11 December, 2004
[12] M Koshiba, *J. Lightwave Technol.* **19**, 1970 (2001)
[13] A Martinez, F Cuesta and J Marti, *Photonics Technol. Lett.* **15**, 694 (2003)
[14] Y Nagpal and R K Sinha, *Microwave Opt. Technol. Lett.* **43**, 47 (2004)