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Execution Date: 6 Feb 2003

4. Application number(s) or patent number(s):
If this document is being filed together with a new application, the execution date of the application is: __

Title: PHOTONIC BAND GAP MATERIALS BASED ON SQUARE SPIRAL POSTS IN A TETRAGONAL LATTICE

A. Patent Application No.(s)
09/988,386 filed 11/19/2001

B. Patent No.(s)

Additional numbers attached? ____ Yes X No

5. Name and address of party to whom correspondence concerning document should be mailed:
Name: Ralph A. Dowell
Internal Address: _____
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6. Total number of applications and patents involved: 1

7. Total fee (37CFR 3.41).....$ 40.00

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ASSIGNMENT OF RIGHTS TO THE UNIVERSITY OF TORONTO BY THE INVENTOR

In consideration of the sum of two dollars ($2.00) and other good and valuable consideration, the receipt and sufficiency of which are hereby acknowledged, **Sajeev John,** and **Ovidiu Toader,** their heirs, executors, administrators and assigns (collectively the "Assignor") hereby sell, assign and transfer to The Governing Council of the University of Toronto, its successors and assigns (collectively the "Assignee") all right, title and interest which the Assignor now has or may hereafter have in an invention described as

Photonic Band Gap Materials Based on Square Spiral Posts in a Tetragonal Lattice

in Appendix A annexed hereto, (the "Invention")

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Executed at Toronto, Ontario this 6th day of February, 2003.

Witness

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Ovidiu Toader

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UNIVERSITY OF TORONTO CONFIDENTIAL INVENTION DISCLOSURE

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1. Title of Invention

PHOTONIC BAND GAP MATERIALS BASED ON SQUARE SPIRAL POSTS IN A TETRAGONAL LATTICE

2. Inventors

SURNAME, GIVEN NAMES	UNIVERSITY PERSONNEL NO.	DEPARTMENT (LIST ANY CROSS APPOINTMENTS OR AFFILIATED INSTITUTIONS)	AFFILIATION WITH UNIVERSITY (i.e. FACULTY, ASSOC., STUDENT, STAFF, VISITOR, etc.)	UNIVERSITY ADDRESS, PHONE, FAX, EMAIL
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TOADER, OVIDIU		PHYSICS	GRADUATE STUDENT	978 5444 OVI@PHYSICS.UTORONTO.CA

3. Description of Invention

(Please highlight the novelty/patentable aspect; attach more detailed description)

This invention provides a complete theoretical blueprint for a new class of photonic band gap (PBG) materials which can be readily synthesized using glancing angle deposition (GLAD) and infiltration of high refractive index semiconductors such as silicon or germanium. The resulting
PBG can be roughly 25% (compared to only 5-9% for the inverse opals) and is very robust to disorder effects. This is nearly the size of the PBG envisioned in the inverse diamond structure, but is much easier to synthesize than the diamond structure. Both the post structure and the inverse post structure have large gaps. The gap occurs between the 4th and 5th bands in
the photonic band structure and is distinct from any previously considered PBG material

DATE RECEIVED: JUL 0 4 2000 **DISCLOSURE REFERENCE NO.:** RIS 10000658
(For Research Services use only)

4. **How was the research funded?**

SPONSOR	GRANT OR CONTRACT FUND #	INTELLECTUAL PROPERTY TERMS & CONDITIONS
NSERC	415174	

5. **Where was the research carried out?**

UNIVESITY OF TORONTO

6. **Is the invention related to any Material Transfer, Confidentiality or Non-Disclosure Agreement?**

◉ **NO** ○ **YES** (If "Yes", please provide details)

7. **Has the invention been publicly disclosed? Will it be soon?**

(Please give details)

NO DISCLOSURE YET. A U.S. RPOVISIONAL PATENT APPLICATION WILL BE FILED FOLLOWED BY A PUBLICATION IN A MAJOR SCIENCE JOURNAL.

8. **What are the potential application(s)?**

OPTICAL TELECOMMUNUCATIONS AND OPTICAL COMPUTING

9. **Warranty**

I/We have read, understood and agree to all of the preceding and declare that all of the information provided in this disclosure is complete and correct. To the best of our knowledge, all persons who might legally make an ownership claim on this invention are identified in Section 2.

Signature _____ Date _____
Typed Name: SAJEEV JOHN JULY 4, 2000

Signature _____ Date _____
Typed Name:

Signature _____ Date _____
Typed Name: OVIDIU TOADER July 4, 2000

Signature _____ Date _____
Typed Name:

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HILL & SCHUMACHER

Title: PHOTONIC BAND GAP MATERIALS BASED ON SQUARE SPIRAL POSTS IN A TETRAGONAL LATTICE

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TITLE

FIELD OF THE INVENTION

The present invention relates to photonic band gap materials and more specifically, it describes a photonic crystal structure which generates a stable and relatively large full photonic band gap. The crystal can be fabricated using the Glancing Angle Deposition (**GLAD**) method.

BACKGROUND OF THE INVENTION

Photonics is the science of molding the flow of light. Photonic band gap (**PBG**) materials, as disclosed in S. John, Phys. Rev. Lett. 58, 2486 (1987), and E. Yablonovitch, Phys. Rev. Lett. 58, 2059 (1987), are a new class of dielectrics which carry the concept of molding the flow of light to its ultimate level, namely by facilitating the coherent localization of light, see S. John, **Phys. Rev. Lett**. 53, 2169 (1984), P. W. Anderson, **Phil. Mag.** B 52, 505 (1985), S. John, **Physics Today** 44, no. 5, 32 (1991), and D. Wiersma, D. Bartolini, A. Lagendijk and R. Righini, **Nature** 390, 671 (1997). This provides a mechanism for the control and inhibition of spontaneous emission of light from atoms and molecules forming the active region of the PBG materials, and offers a basis for low threshold micro-lasers and novel nonlinear optical phenomena. Light localization within a PBG facilitates the realization of high quality factor micro-cavity devices and the integration of such devices through a network of microscopic wave-guide channels (see J. D. Joannopoulos, P.R. Villeneuve and S. Fan, **Nature** 386, 143 (1998)) within a single all-optical microchip. Since light is caged within the dielectric microstructure, it cannot scatter into unwanted modes of free propagation and is forced to flow along engineered defect channels between the desired circuit elements. PBG materials, infiltrated with suitable liquid crystals, may exhibit fully tunable photonic band structures [see K. Busch and S. John, **Phys. Rev. Lett.** 83, 967 (1999) and E. Yablonovitch, **Nature** 401, 539 (1999)] enabling the steering of light flow by an external voltage. These possibilities suggest that PBG materials may play a role in photonics, analogous to the role of semiconductors in conventional microelectronics. As pointed out by Sir John Maddox, "If only it were possible to make dielectric materials in which electromagnetic waves cannot propagate at certain frequencies, all kinds of almost magical things would be possible." John Maddox, **Nature** 348, 481 (1990).

Building three dimensional photonic crystals with band gaps centered at a wavelength shorter than 2 microns poses a great challenge. The microscopic structure of such a crystal should generate a large gap and in the same time lend itself to micro-fabrication. GLAD method [see K. Robbie and J. Brett, **Nature** 384, 616 (1996)] is a relatively new technique which has

been used to successfully engineer three dimensional thin film micro-structures on sub micrometer scales. Complex three dimensional structures can be fabricated by combining oblique vapor deposition and substrate motion. Examples of structures already created can be found in Fig. 1 and the following references: K. Robbie and J. Brett, **J. Vac. Sci. Technol. B** 15, 1460-1465 (1997) and K. Robbie, J. C. Sit and J. Brett, **J. Vac. Sci. Technol. B**, 16, 1115-1122 (1998).

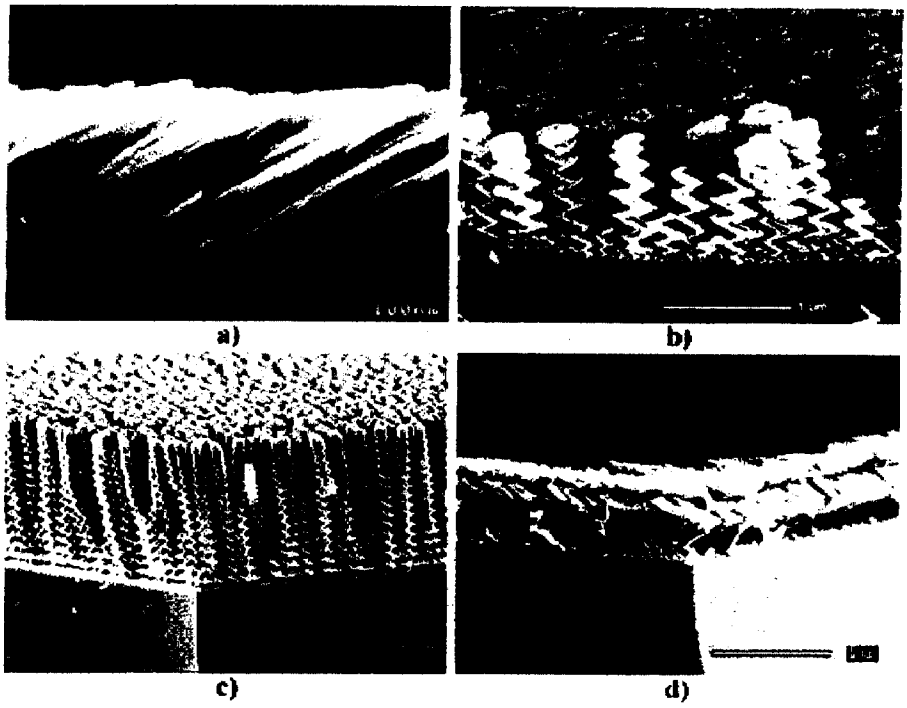


Fig.1 : http://physics.queensu.ca/~robbie/glad.html

In short GLAD is based on thin film deposition, by evaporation or sputtering, and employs oblique angle deposition flux and substrate motion to allow nanometer scale control of structure in engineered materials. The substrate is oriented at a large oblique angle relative to the incident vapor flux. This leads to an effect called atomic shadowing and results in a porous structure with isolated columns of material growing toward the vapor source. Semiconductors, metals, metal oxides and fluorides can be used by GLAD. The microstructures built using GLAD can be used as templates for growing structures from an even larger range of materials.

SUMMARY OF THE INVENTION

In this document we present a detailed description of the electromagnetic properties of a 3d photonic crystal with a novel architecture. The structure of this photonic crystal enables the generation of a stable and relatively large full photonic band gap. We describe the structure of the photonic crystal in terms of a set of geometrical parameters and we find the optimum set of

parameters for which the maximum full photonic band gap can be realized. It is found that in the case of Si used as the high dielectric material the "direct structure" (to be explained below) possesses a 15% full photonic band gap and the "inverted structure" possesses a 23% full photonic band gap. The glancing angle deposition method can be used for fabricating this type of photonic crystals.

DETAILED DESCRIPTION OF THE INVENTION

The object of our invention is a photonic crystal whose structure is depicted in Fig.2. The geometry of the building blocks of the crystal is described in Fig.3. The underlying lattice of the crystal is tetragonal with lattice constants c along the z axis and a along x and y axes. In the description below we choose to express all the lengths in terms of a.

The structure of the crystal

The building block of the crystal is made from a coil of pitch c (see Fig.3 Side view) with a single loop whose transverse cross section is a square with edge of length L (see Fig.3 Top view). The pitch is the same as the lattice constant and the coil is wrapped around the z axis. Each of the segments of the coil is coated with a cylinder of radius r (see Fig. 3 Top view) whose dielectric constant is denoted by ε_s. The spirals are embedded in a material whose index of refraction is ε_b. In our exploration of the parameters space we impose no restriction on the size of L relative to a and allow for overlapping between adjacent spirals.

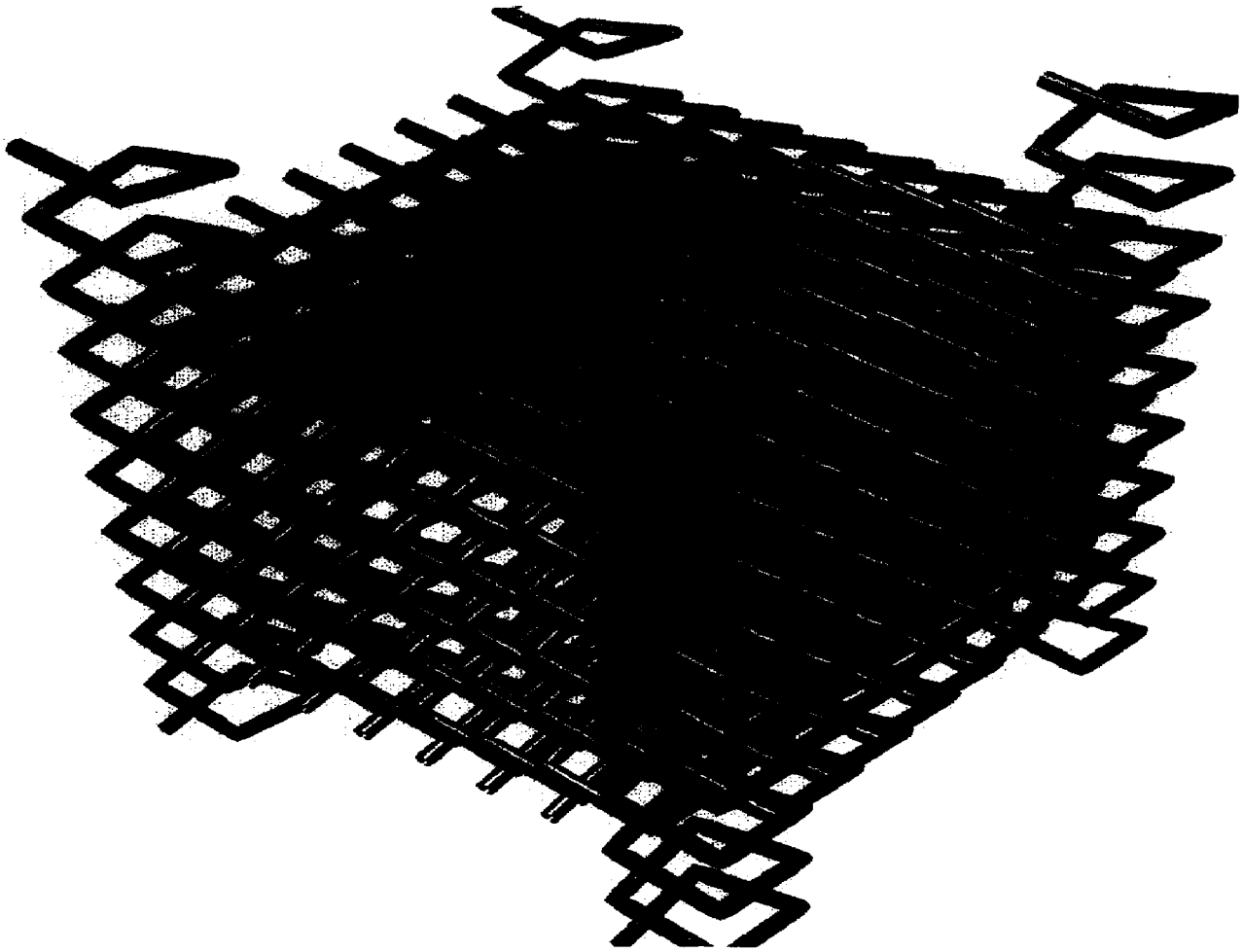


Fig.2 A piece of the ''Square spirals" photonic crystal. In order to make the image clearer the spirals at the corners of the crystal are highlighted with a different color and size. All the spirals have the same geometry.

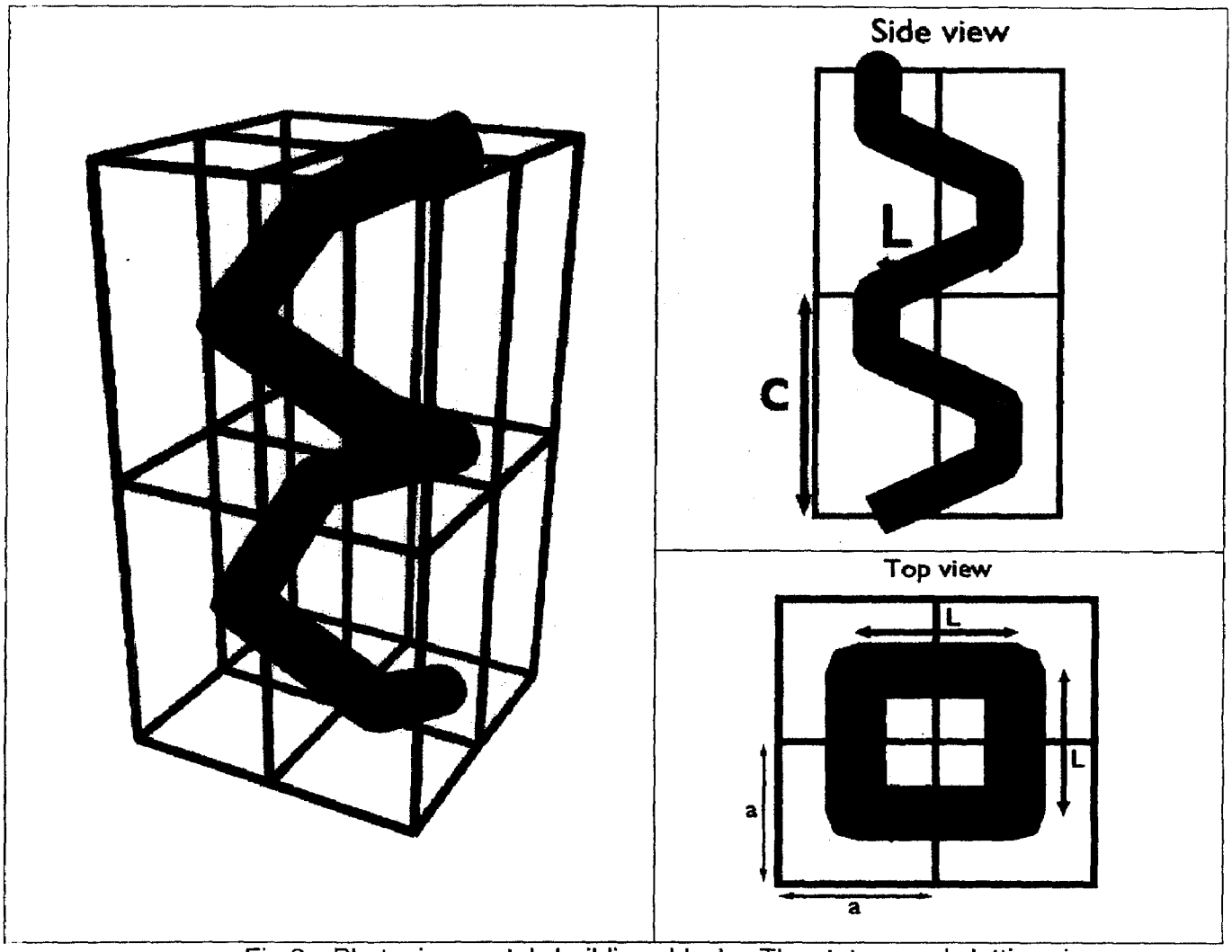


Fig.3. Photonic crystal building block. The tetragonal lattice is characterized by lengths a and c. The geometry of the square spiral is characterized by its width, L radius, r and pitch c. For clarity a single spiral is shown coiling around in 4 unit cells.

For the theoretical modeling of the electromagnetic properties of the photonic crystal we will use a value of 11.9 for the dielectric constant of the material with high index of refraction. This approximates very well Si at wavelengths around 2 microns (see Edward D. Palik, **Handbook of Optical Constants of Solids**, Academic Press Inc., Orlando, 1985). The **direct structure** crystal is defined by $\varepsilon_b = 1$, $\varepsilon_s = 11.9$ and the **inverted structure** crystal is defined by $\varepsilon_b=11.9$, $\varepsilon_s=1$. In our analysis we choose to treat only the tetragonal Bravais lattice because both the face centered cubic, or body centered cubic lattices require a c/2 translation along the z axis between adjacent spirals and we believe that this cannot be controlled by the GLAD technique as it stands today.

In **Phys. Rev. B**, 57, 2006-2008 (1998) the authors study photonic crystals built from circular spiral elements on simple cubic, face centered cubic and body centered cubic lattices. It is reported that in the case of a crystal made from a material with a dielectric constant of 12.25 (the spirals) in air the maximum band gap is only 3 % and it appears when the simple cubic lattice is deformed into a tetragonal lattice. We believe that both the structure of the spirals (square in our study) and the fact that they overlap contribute to the significant enhancement of the size of the full photonic band gap in the case of our crystal structure.

In the theoretical calculations we have used the plane waves expansion method (see **Phys. Rev. Lett.**, 65, 3152-3155 (1990)) for calculating the photonic band structure of the crystal. For all of the calculations we have used an expansion with more than 1400 plane waves. The Fourier coefficients of the dielectric have been calculated using the Fast Fourier Transform method with a sampling of at least 512^3 points in one unit cell.

The theoretical calculations for both the direct and inverted structures are presented in the following two sections.

Direct Structure

The direct structure photonic crystal is characterized by ε_s=11.9 and ε_b=1 and all the geometrical parameters described in Fig. 3. In this case we find a local maximum of the relative band gap as a function of L, r and c for the combination **[L,c,r] = [1.6,1.2,0.14]**. All these parameters are measured in units of a, the lattice constant.

The filling factor of the spirals, f_{spir}, serves as a measure of the degree with which the spirals form a connected or disconnected structure. At small f_{spir} the individual spirals are disconnected and the air forms the connected component in the system whereas for largef_{spir} both the air and spirals form connected components. The calculations show that a sizable full photonic bad gap exists for a wide range of spirals filling factor.

In Fig.4 we show the photonic band structure and the position of the high symmetry points in the Brillouin zone for the direct structure crystal with the optimized parameters. A large photonic band gap of relative width 15.2 % opens between 4-th and 5-th bands. The upper edge of the photonic band gap closes at R point and only two bands, 5-th and 6-th, contribute to the spectrum around the upper edge, thus a large pseudogap is expected in this spectral region.

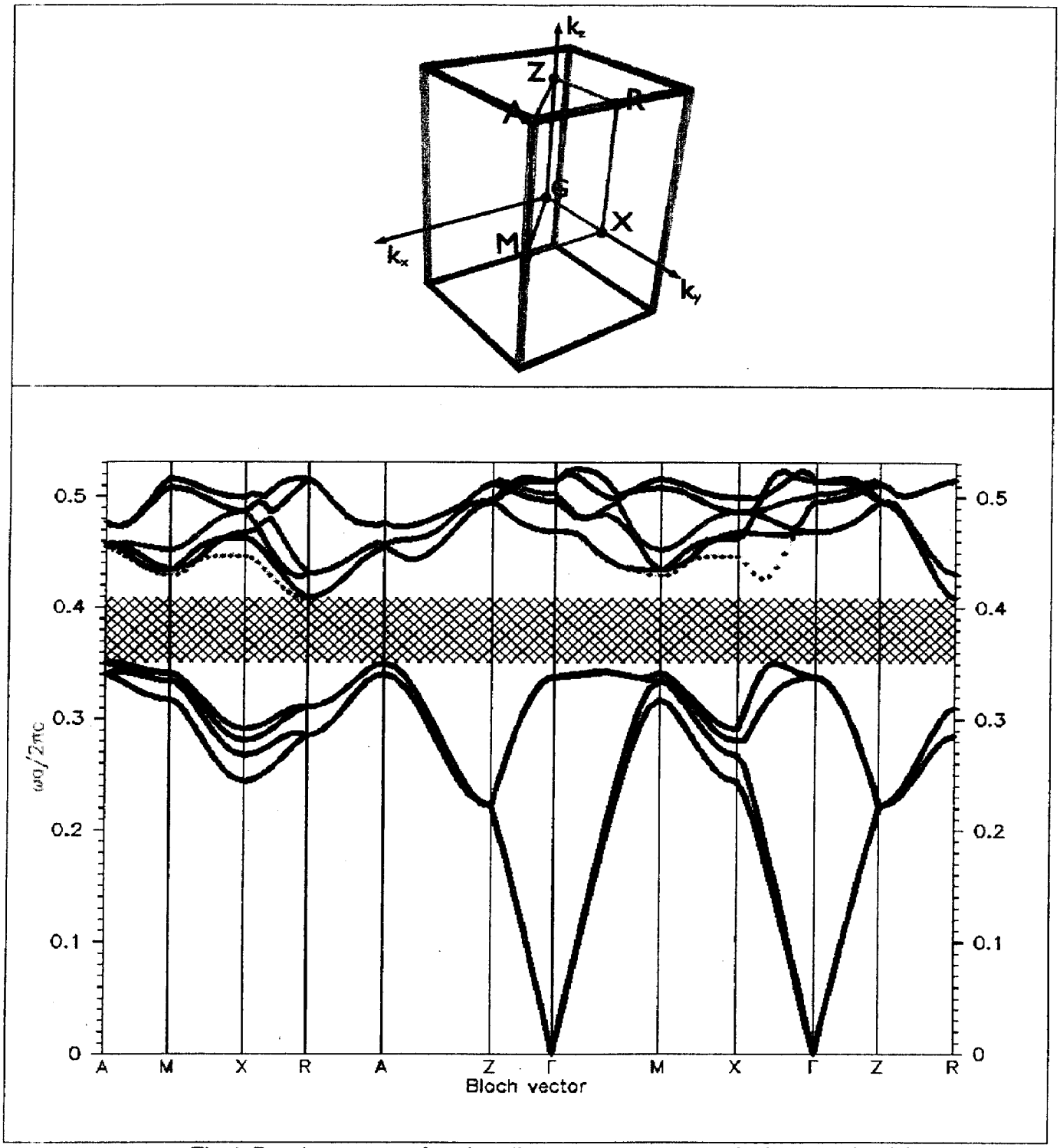


Fig.4 Band structure for the direct structure crystal characterized by **[L,c,r] = [1.6,1.2,0.14]** . The lengths are given in units of a, the lattice constant. The relative width of the photonic band gap is 15.2%. The positions of high symmetry points are illustrated in the top figure where G stands for Γ.

In Fig.5 we show the total density of states for the direct structure crystal whose band structure is shown in Fig.4. In our calculation we used the improved tetrahedron method [see **Phys. Rev. B**, 49, 16223-16233 (1994)] adapted to the photonic case. The large pseudogap around the full band gap has a relative width of 25.5%.

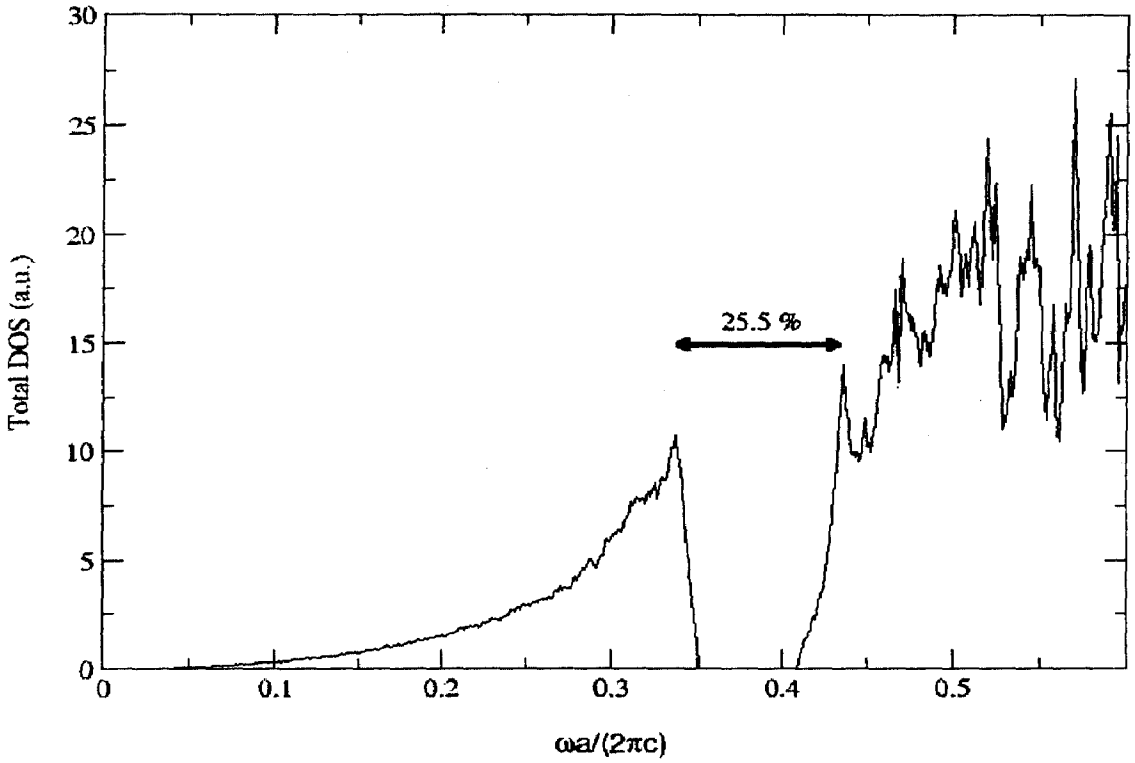


Fig 5 Total density of states for the direct structure optimized crystal characterized by **[L,c,r] = [1.6,1.2,0.14]**. The lengths are given in units of a, the lattice constant. The density of states is measured in arbitrary units.

Fig.6 displays the relative width of the full gap as a function of r and c for a fixed L=1.6 for the direct structure crystal. The value of L was chosen to optimize the size of the gap. It is found that the variation of the size of the gap with the geometry of the spirals is relatively slow in the region around the maximum. Constant value contours are shown on the plot to better illustrate this point. The filling fraction of the spiral component varies from 14% to 40% over the range of parameters shown in the plot.

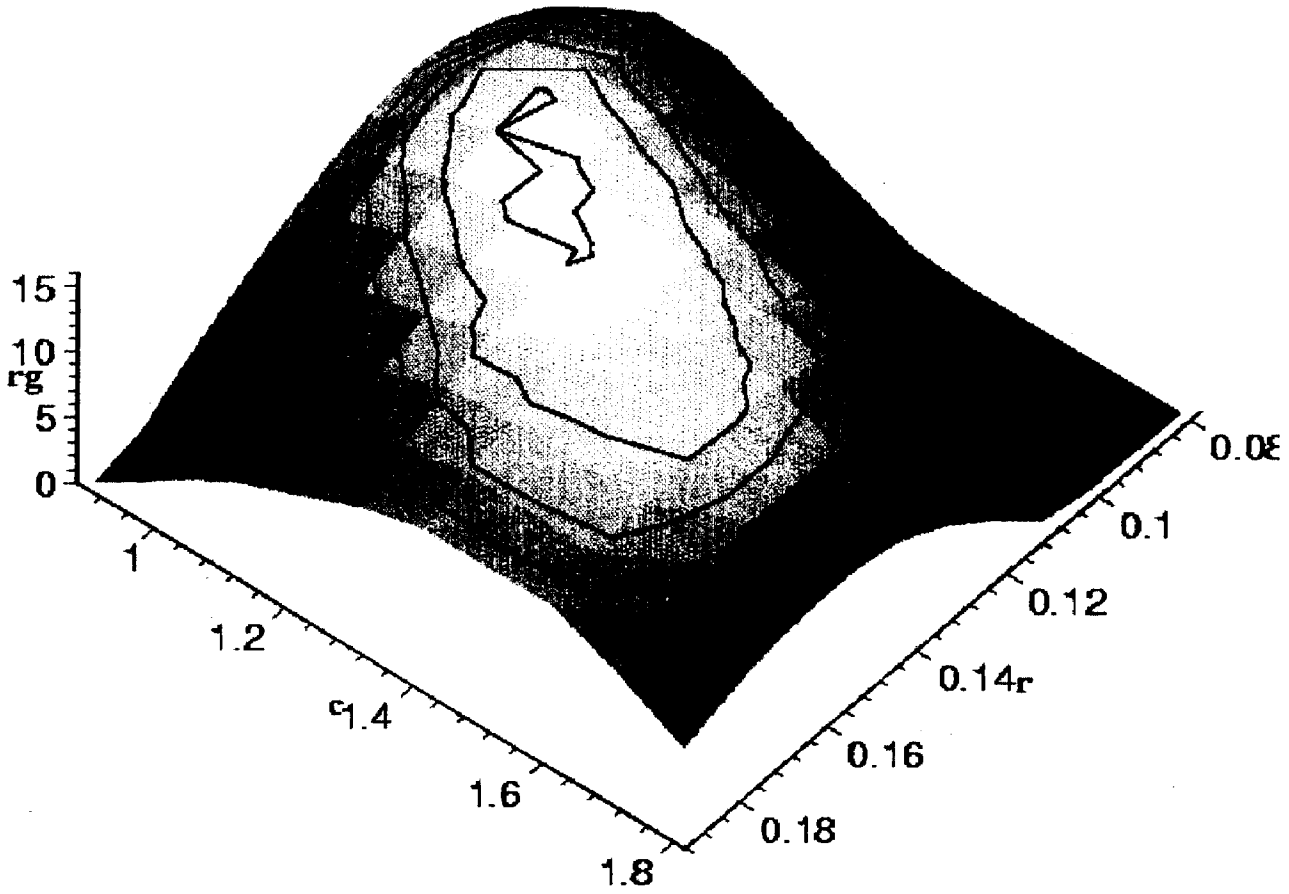


Fig 6 Relative gap, **rg** (measured in %) as a function of r and c for L=1.6 for the direct structure crystal. Constant value contours are also sketched on the plot for all the integer values from 1 to 15. The maximum value is 15.2 %.

Fig 7 shows the relative size of the gap as a function of the spirals filling fraction for L=1.6 and various values of c. When L and c are fixed the spirals filling fraction is a function of r only. The curves show that the optimum f_{spir} is around 25%.

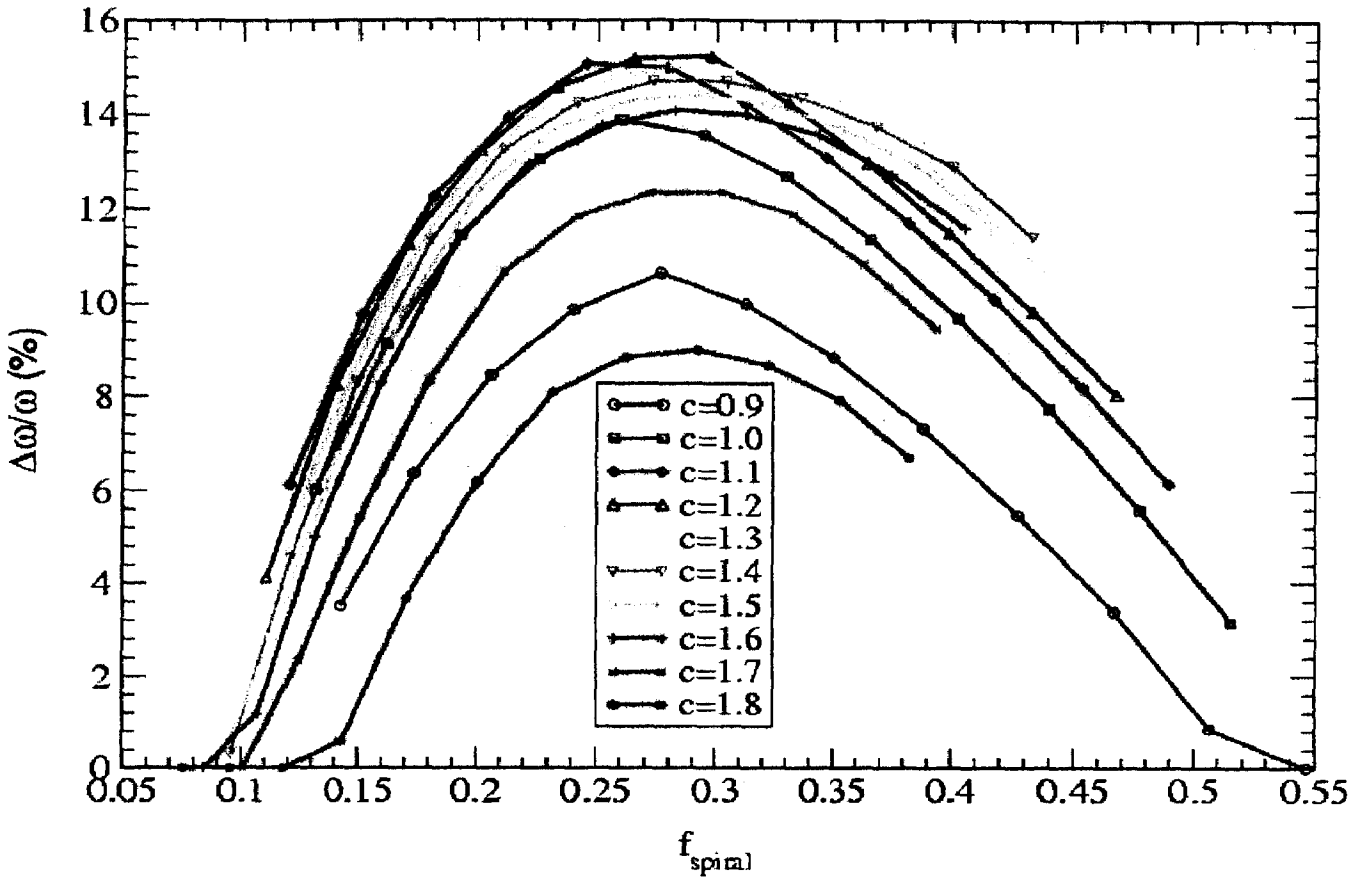


Fig 7 Relative gap of the direct structure crystal as a function of f_{spir} for L=1.6. Different curves correspond to different values for c.

The spatial distribution of the electromagnetic field in the photonic crystals is also of great interest. The ability to alter the coupling between the matter and radiation field in the photonic crystal is influenced dramatically by the electric field at the specific location [see **Phys. Rev. E.**, 58, 3896-3908 (1998)]. In Fig. 7.1 we show the spatial distribution of the absolute value of the electric field for the mode corresponding to the 5-th band at the R point. The region sampled contains a few units cells (the unit of length is again a). The figure shows three slices each perpendicular to the x, y and z axes. The electric field is calculated on each of the three slices and its absolute value is used as the color function (See the color bar). The dielectric constant is sampled as well on the same planes and its value is used to warp linearly the surface of the slice. The deformation is 0 where the dielectric constant is minimum (air in this case) and has an arbitrary value in the high dielectric component (spirals in this case). The deformation of the plane perpendicular to the x axis is in the positive x direction and similarly for the planes perpendicular to y and z axes.

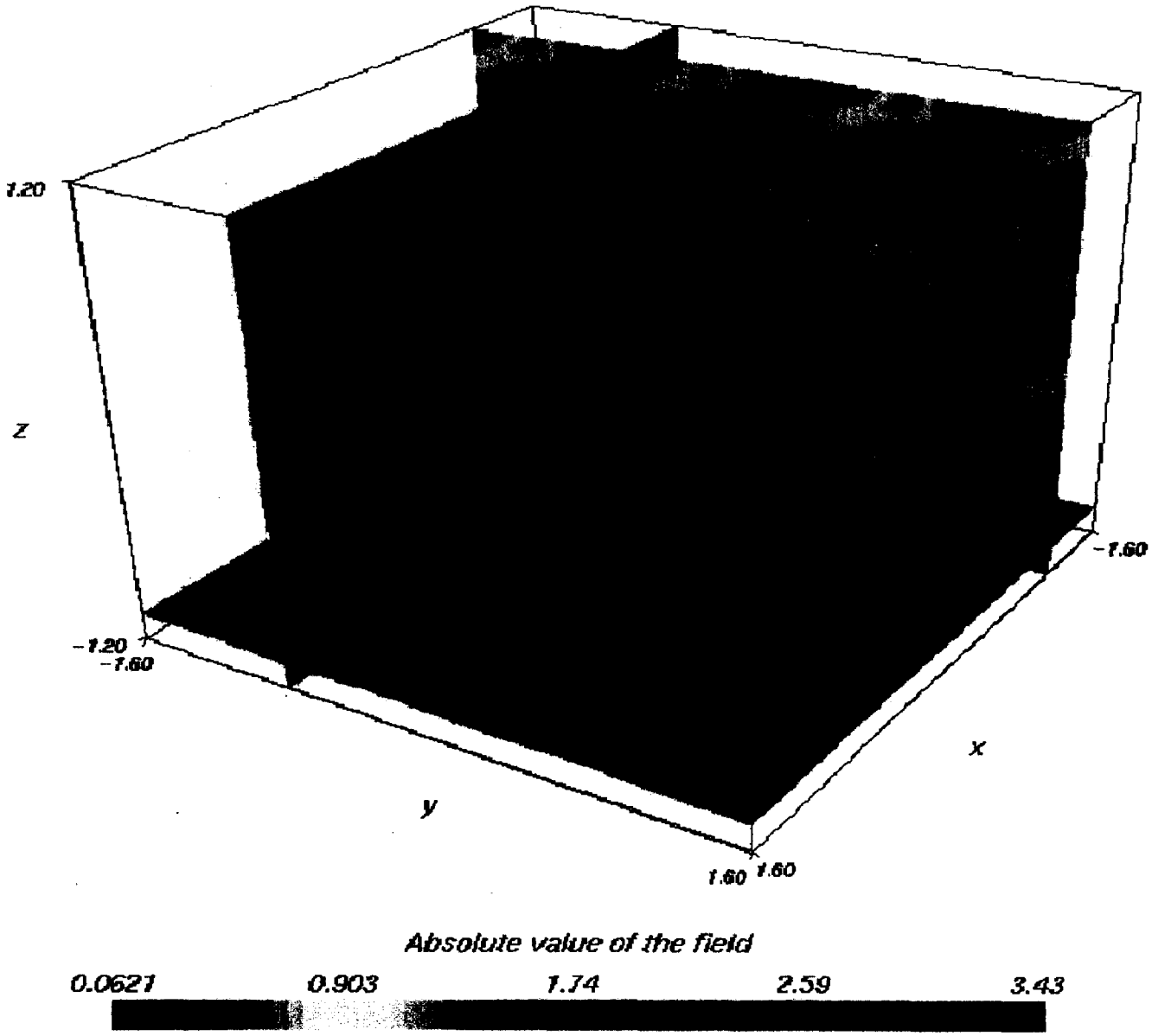


Fig. 7.1 Absolute value of the electric field for the mode corresponding to the 5-th band at R point (Fig. 4). The absolute value of the E field is color coded according to the color bar. The dielectric constant is represented by the relief of the slice plane. The deformation of the slice plane is proportional to the dielectric constant with 0 deformation where the dielectric constant is minimum.

Inverse structure

Similar calculations have been performed for the inverted structure crystal, characterized by ε_b=11.9 and ε_s=1. In this case we find a local maximum of the relative band gap as a function of

L, r and c located at **[L,c,r] = [1.5,1.7,0.33]**. In Fig.8 we show the photonic band structure and of the inverse structure crystal with the optimized parameters. A large photonic band gap of relative width 23.6 % opens between 4-th and 5-th bands.

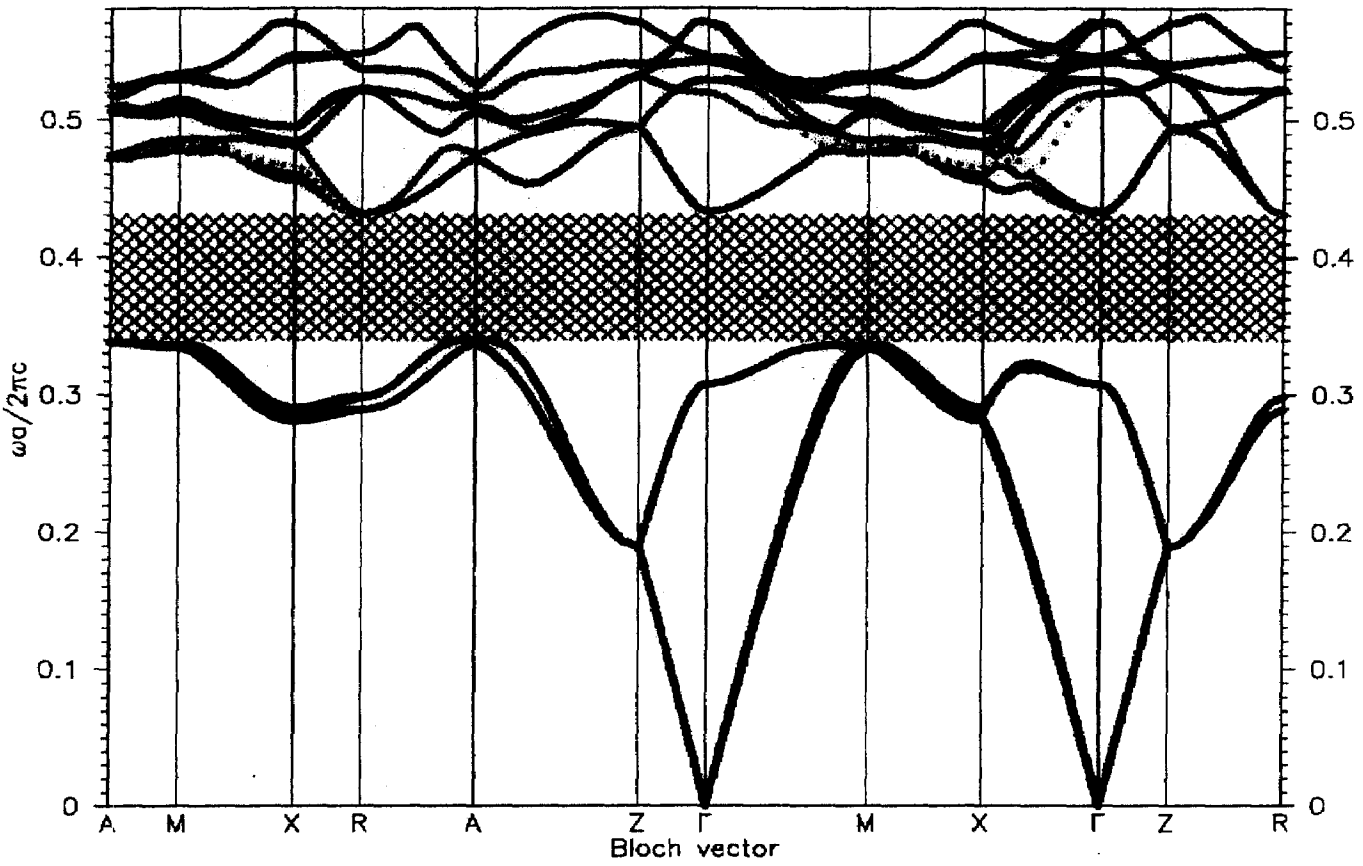


Fig. 8 Band structure for the inverse structure crystal characterized by **[L,c,r] = [1.5,1.7,0.33]**. The lengths are given in units of a, the lattice constant. The relative width of the photonic band gap is 23.6 %. The positions of high symmetry points are illustrated in Fig 4.

In Fig. 9 we show the total density of states for the inverse structure crystal whose band structure is shown in Fig. 8. It is worth mentioning the fact that in the case of the inverted structure the size of full photonic band gap is very close to the size of the pseudogap. The fact that both the lower and upper edges of the full photonic band gap close at two symmetry points (lower edge at A and M points and the upper edge at Γ and R) explains this optimal full photonic band gap.

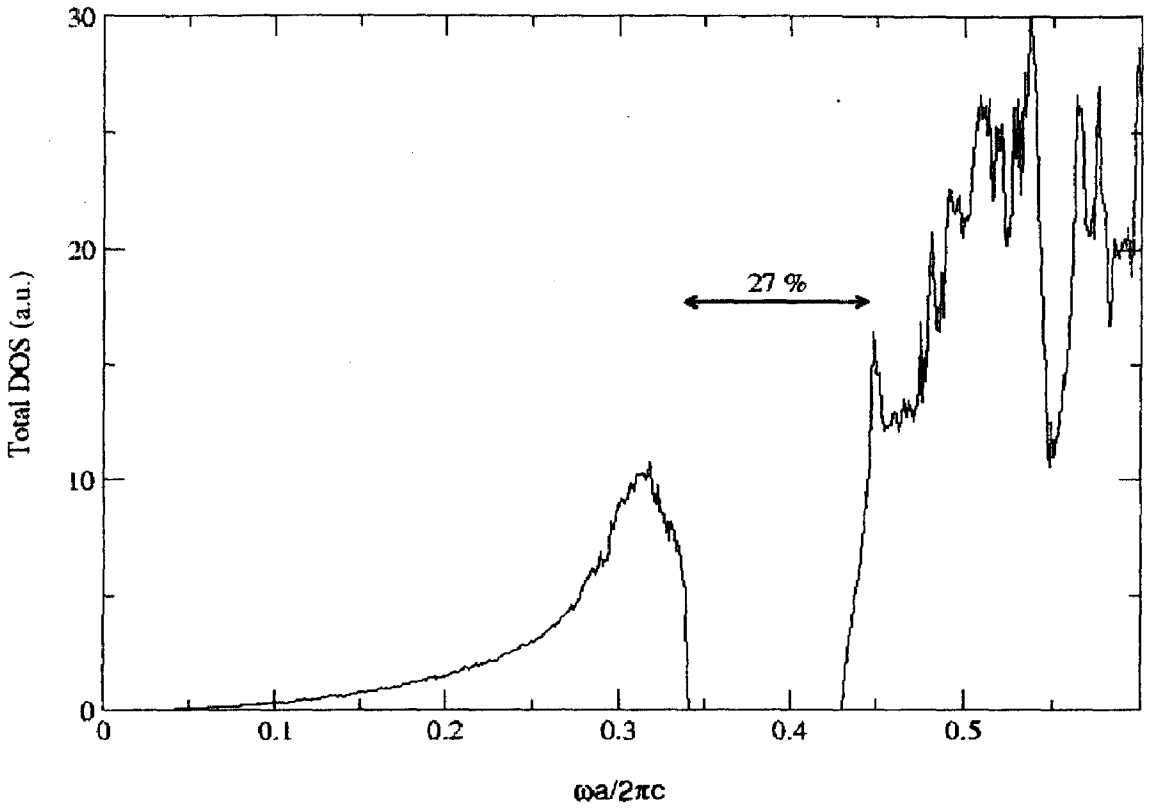
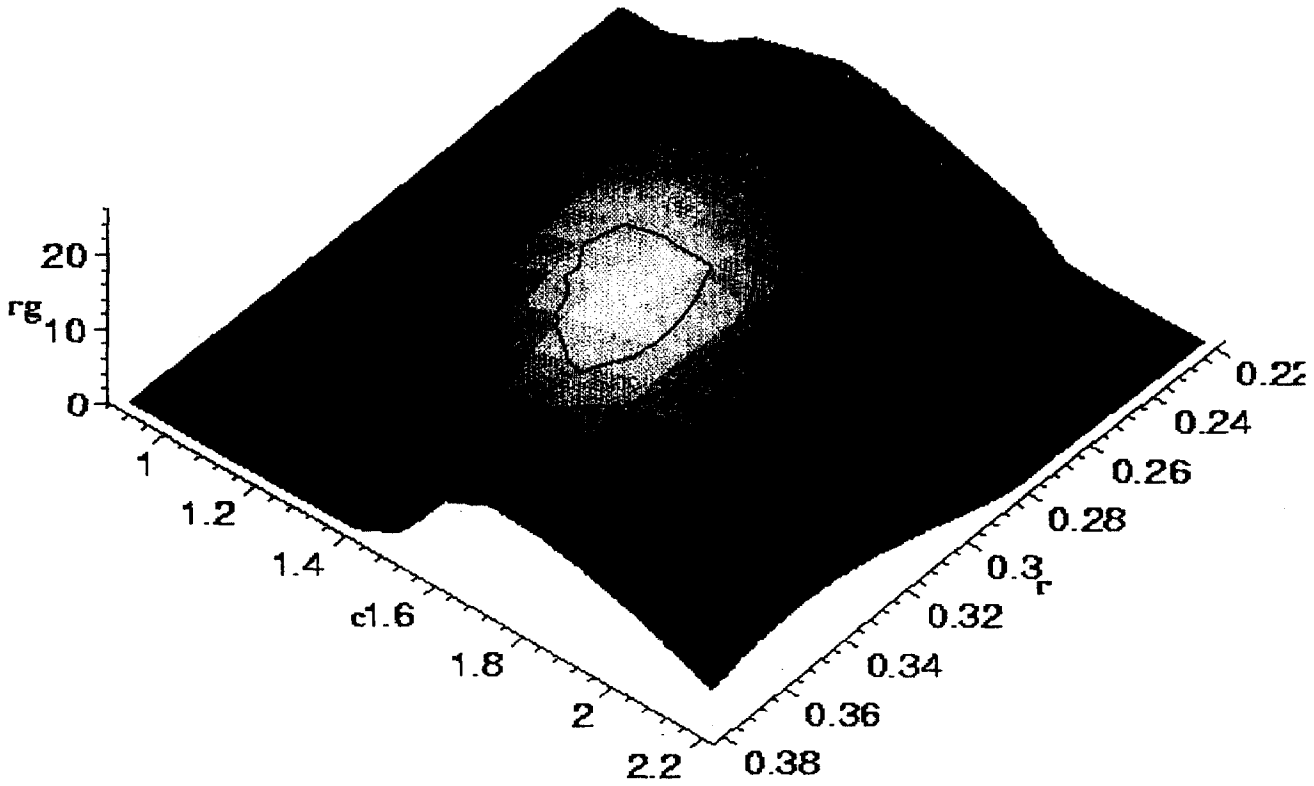


Fig. 9 Total density of states for the inverse structure optimized crystal characterized by **[L,c,r] = [1.5,1.7,0.33]**. The lengths are given in units of a, the lattice constant. The density of states is measured in arbitrary units.

Fig. 10 displays the relative width of the full gap of the inverse structure crystal as a function of r and c for a fixed L=1.5. The value of L was chosen to optimize the size of the gap. It is found that the variation of the gap with the geometry of the spirals is relatively slow in the region around the maximum. Constant value contours are shown on the plot to better illustrate this point. The filling fraction of the higher index of refraction component of the optimized crystal is 21%.



Relative gap, **rg** (measured in %) as a function of r and c at L=1.5 for the inverse structure crystal. Constant value contours are also sketched on the plot. The maximum value of the relative band gap is 23.6 %.

THEREFORE WHAT IS CLAIMED IS:

The **Square Spirals** photonic crystal possesses the qualities of a very good photonic crystal. Both the direct and inverted structures have a large full photonic band gap which is stable with respect to the changes in the crystal's geometrical parameters.

For both the direct and inverted structures we found a set of geometrical parameters which can be used for fabricating such a photonic crystal with the optimum full photonic band gap.

The topological structure of the crystal facilitates the transport of atomic or molecular beams and can serve very well as the basis of active devices based on the Quantum Optical properties of the photonic crystals where the interaction between matter and the special electromagnetic modes inside such a photonic crystal can be exploited.