Theoretical investigation of fabrication-related disorder on the properties of photonic crystals

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How various deviations in perfect photonic crystals, which may arise during fabrication, can affect the size of photonic band gaps is investigated theoretically. The emphasis is on determining the effects of misalignment of basic structural elements and overall surface roughness, because of their general fabrication relevance. As an example, calculations on a newly proposed three-dimensional photonic crystal are performed. It is shown that the size of the gap is tolerant to significant amounts of deviation from the perfect structure. © *1995 American Institute of Physics.*

I. INTRODUCTION

Photonic band-gap (PBG) materials have emerged as a potentially new class of materials for the fabrication of optoelectronic devices.[1,2] By suppressing all modes within the frequency gap, PBG materials can greatly affect the radiative dynamics within the structure and lead to significant changes in the properties of optical devices. One limiting factor for the use of these materials has been associated with their fabrication. Small deviations may arise during the fabrication process and affect the properties of PBG materials. The effects of uniform deviations arising from a systematic change of structural elements have been considered in several structures.[3–8] In this paper, we choose to study disorder most likely to arise during fabrication, such as surface roughness and misalignment of the dielectric components. We are interested in their effects on the most fundamental property of photonic crystals: the size of the gap.

For concreteness, we focus on a three-dimensional PBG crystal proposed recently as a viable structure for fabrication at micron and submicron length scales.[8] The perfect crystal structure is shown in Fig. 1. It is essentially a layered structure, typical of most 3D photonic crystals at these length scales.[5–8] One possible fabrication process of this structure is illustrated in Fig. 2 and described briefly below. It is presented here to help readers grasp the relationship between the basic structural elements. A detailed discussion of this fabrication process can be found elsewhere.[8]

The structure is fabricated by first depositing a layer of dielectric material of thickness h onto a substrate and by etching long parallel grooves into the layer along the x-axis. The grooves are separated by a distance a and have a depth d and width w. The grooves are then backfilled with a second dielectric material, and another layer of the first material is grown on the surface, as shown in Fig. 2(a). Long grooves are then etched into this top layer, translated by a distance $a/2$ with respect to those in the first layer. After backfilling the grooves with the second dielectric, the entire process is repeated several times such that the structure repeats itself every other layer, as shown in Fig. 2(b). Once this process is completed, the second dielectric material, if properly chosen, can be removed from the structure with selective etching, as shown in Fig. 2(c). An array of long cylindrical holes is then etched into the top surface of the structure, at normal incidence. The holes are separated by a distance b and the x-axis and a along the y-axis. The center of each hole is aligned in the structure as shown in Fig. 2(d). In the case of a perfect structure, the complete gap can be as large as 23% using materials such as Si or GaAs. The maximum gap is reached when $h=0.35a$, $b=0.71a$, $d=0.51a$, and $w=0.36a$.[8]

The size of the gap will most likely be reduced by any structural deviation from the perfect crystal. But it is of practical relevance to analyze the consequences of disorder arising naturally in the fabrication process at micron and submicron length scales. Such disorder includes overall surface roughness and misalignment of the basic elements. Since the structure described above is essentially a layered structure, its fabrication is carried out in stages. While the position of the basic elements and their shape and dimension can be controlled to high accuracy at each stage, keeping the uniformity between stages is more challenging. We therefore choose to study the following fabrication-related disorders:

(i) variations of layer thickness,
(ii) variation of groove depth,
(iii) misalignment of grooves between layers,
(iv) inaccuracy in fabricating air columns,
(v) overall surface roughness.

The actual size of the disorder will depend on the precision of the lithographic technique used in the fabrication process, and the relative size of the disorder to the minimum feature size of the photonic crystal will depend on the midgap frequency for which the photonic crystal is designed. The higher the frequency, the larger the ratio of disorder to minimum feature size for a given technique. A photonic crystal designed for 1.55 μm light will have a minimum feature size of about 0.1 μm. With state-of-the-art x-ray lithographic techniques, feature sizes as low as 0.07 μm can be obtained with a precision between 10% and 20%.[9–11] To be conservative, we have chosen to consider variations of the different features by as much as 57%.

II. COMPUTATIONAL METHOD

To model the various disordered structures, we use the supercell approximation. In this method, a structure containing a specific type of disorder is placed in a large supercell, which is then repeated periodically in position space. Using Bloch's theorem, Maxwell's equations are expanded in a

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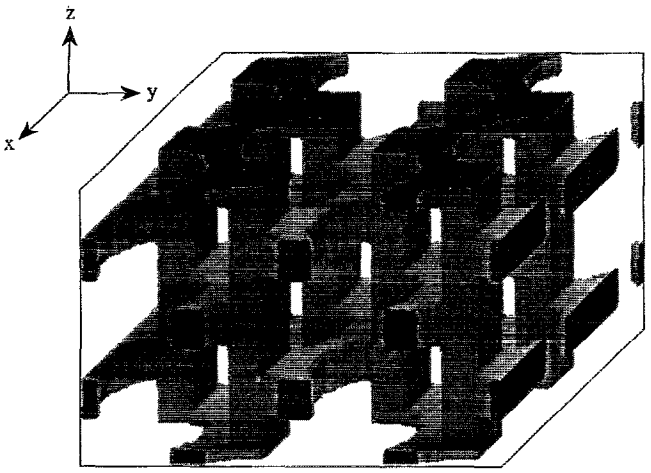

FIG. 1. Perfect three-dimensional photonic crystal fabricatable at submicron length scales. The gray part corresponds to a high index material with the edges shown in black. The rest of the structure is filled with air.

plane-wave basis and transformed into a matrix eigenvalue problem, which is solved by standard numerical techniques. The details of our computational methods are presented elsewhere.[12] In this paper, we use a supercell that contains four layers and eight cylindrical holes, and apply a basis containing 64^3 plane waves which is also equal to the number of real space grid points. We have also tested a smaller supercell and obtained similar results. In any case, the supercell gives a reasonable approximation to the actual photonic crystal, which typically need only be fabricated with ten layers or so.[8] The results of our calculations are presented below.

III. RESULTS

A. Variation of layer thickness

In the perfect structure, each layer has a thickness $h=0.35a$. However, since each layer is grown at a different time, the layers may end up having different thicknesses. We simulate this effect by computing the size of the gap in structures with layers of different thicknesses using the supercell illustrated in Fig. 3. The thickness of each layer is chosen randomly to fluctuate by as much as 20% from that of the perfect structure. We present here results for two different random sets of parameters:

(a) $h_1=0.30a$; $h_2=0.42a$, $h_3=0.30a$, $h_4=0.38a$,

(b) $h_1=0.28a$, $h_2=0.35a$, $h_3=0.42a$, $h_4=0.35a$.

In case (a), the gap is only reduced from 23% down to 21%, while in case (b), it is reduced to 14%. A close examination of the two structures reveals that in case (a), the thinnest horizontal dielectric vein between two grooves has a thickness $h_i+h_{i+1}-d$ of $0.17a$, as opposed to $0.19a$ for the perfect structure. This corresponds to a reduction of the dielectric vein by 11%. In case (b), however, the thinnest vein is reduced by 37% to $0.12a$. Reducing the thickness of this horizontal dielectric vein has the effect of weakening the connectivity of the structure, which is important in opening a photonic band gap.[2]

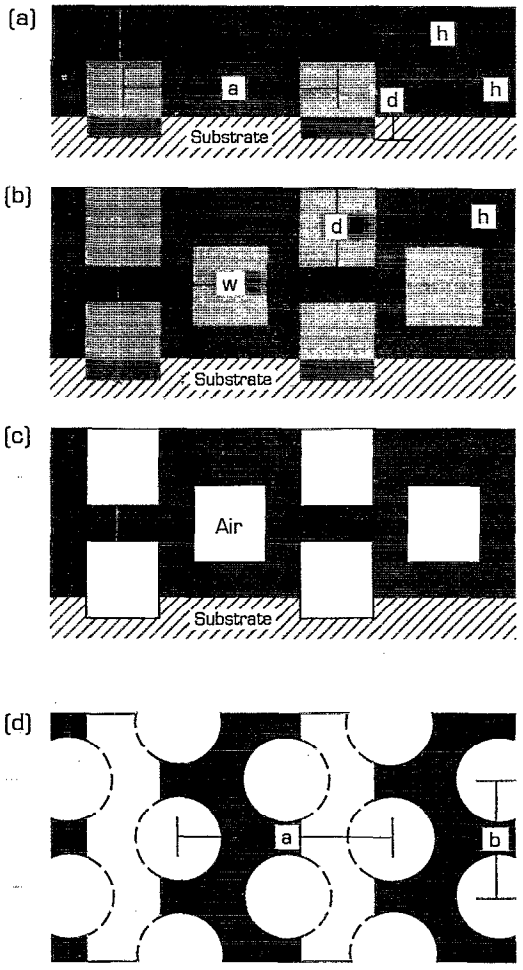

FIG. 2. Generic growth process of the photonic crystal shown in Fig. 1(a)–(c): Cross sectional view in the yz-plane, showing different stages of growth. (d): Plan view in the xy-plane, showing the position of the air holes.

B. Variation of groove depth

In the ideal case, the depth of the grooves is $0.51a$. However, in analogy to thickness variation, the depth of the grooves may also end up having a different value at each step of the fabrication process. We model these changes by using the supercell shown in Fig. 4. Each layer has grooves of the same depth, while different layers have grooves of different depths. The depth of the grooves is chosen randomly to be at most 10% greater or smaller than the one in the perfect structure. Two cases are examined here:

(a) $d_1=0.56a$, $d_2=0.46a$, $d_3=0.46a$, $d_4=0.56a$,

(b) $d_1=0.56a$, $d_2=0.46a$, $d_3=0.56a$, $d_4=0.46a$.

In case (a), the gap is reduced from 23% to 22%, while in case (b), it is reduced to 14%. The thinnest horizontal dielectric vein in case (a) has a thickness $2h-(d_i+d_{i+2})/2$ of $0.19a$, which remains unchanged from that of the perfect structure. In case (b), however, it is reduced by 26% to $0.14a$. In analogy to the effects of thickness variation, these results imply that the size of the photonic band gap is sensitive to the connectivity of the structure.

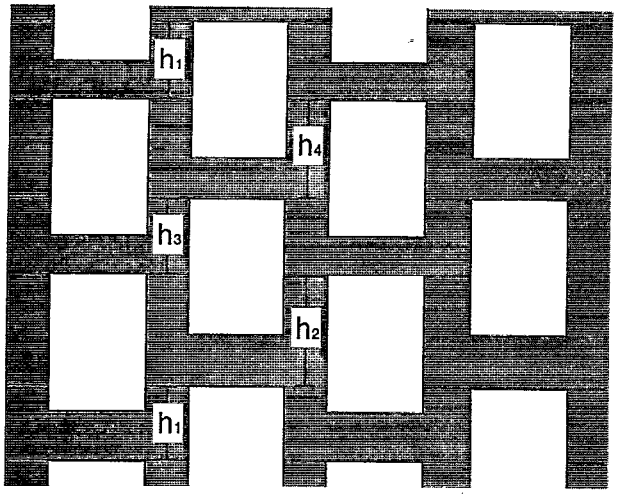

FIG. 3. Cross-sectional view in the yz-plane of a structure with layers of different thicknesses. The structure repeats itself every four layers.

C. Misalignment of grooves between layers

We recall that the structure is made by stacking up layers and by etching a series of grooves within each layer. The grooves are translated by a distance $a/2$ with respect to those in adjacent layers. We are interested in determining the effects of breaking this perfect translational symmetry. We model such disorder by performing computations in the structure shown in Fig. 5. The grooves in the second layer are translated with respect to those in the first layer by a distance l_1, the ones in the third layer with respect to those of the second layer by l_2, and so on. By choosing $l_1=l_2=l_3=l_4=0.5a$, the perfect crystal is reproduced. The minimum feature, which corresponds to the thinnest vertical vein between grooves in neighboring layers, will be significantly affected by any misalignment of the grooves. For example, a misalignment of 16% reduces the minimum feature by more than 57%. In the specific case where $l_1=0.53a$, $l_2=0.52a$, $l_3=0.53a$, and $l_4=0.54a$ (maximum misalignment of 8%), the gap drops to 18.5%, while a structure with $l_1=0.56a$, $l_2=0.54a$, $l_3=0.56a$, and $l_4=0.58a$ (maximum misalignment of 16%) yields a gap of 9.4%. The sensitivity of the gap to the relative position of the grooves is related again to the connectivity of the dielectric network.[2] In the perfect structure, the minimum feature has a size of $0.14a$. In the case where the largest misalignment is 16%, the connectivity of the lattice is weakened since the width of the thinnest vein drops by 57% to $0.06a$. Clearly, great care needs to be taken in this part of the fabrication process. Nevertheless, it is comforting to see that the gap remains respectably large even with such a significant misalignment.

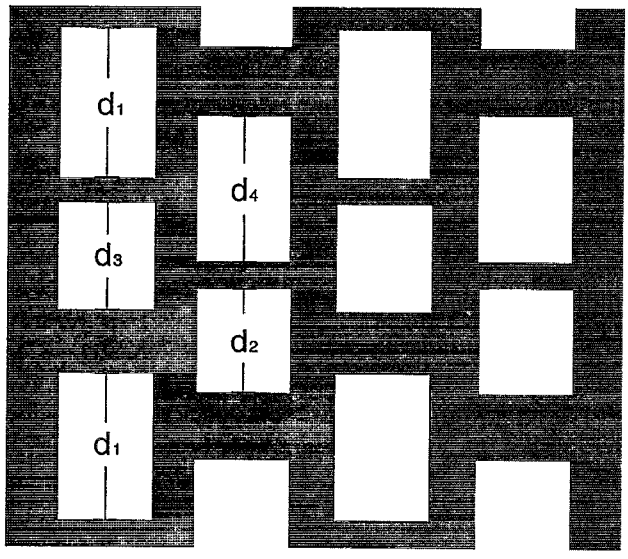

FIG. 4. Cross-sectional view in the yz-plane of a structure with grooves of different depths. The grooves in each given layer have the same depth, but the grooves have different depths in different layers. The structure repeats itself every four layers.

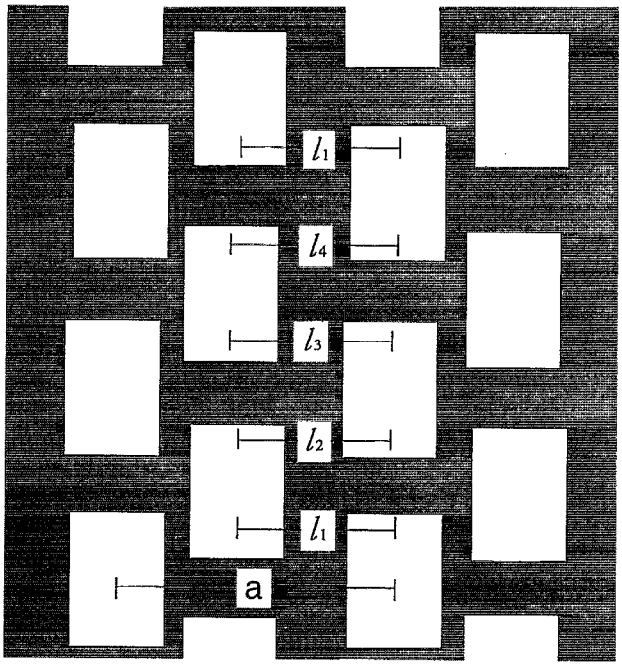

FIG. 5. Cross-sectional view in the yz-plane of a structure with misaligned grooves. The structure repeats itself every four layers.

D. Variations in size and misalignment of air columns

Since all the air columns should be etched at the same time, we first consider the effects of changing the radius of the air columns uniformly. We recall that the size of the gap is largest when the radius of the air columns is $r=0.24a$. The gap remains larger than 20% for any uniform change of the radius throughout the structure from $0.21a$ to $0.26a$. Next we consider the effects of misaligning the mask. In the perfect structure, the center of each column should be placed at the midpoint between nearest neighbor grooves. However, during fabrication, the mask may not be perfectly aligned with the wafer. Any misplacement of the mask along the x-axis will have no effect on the overall features of the photonic crystal. Hence we may investigate only the effects of misplacement along the y-axis. In addition to the misplacement of the mask, the perfect lattice of air holes may also be broken. We model these deviations by setting up a supercell

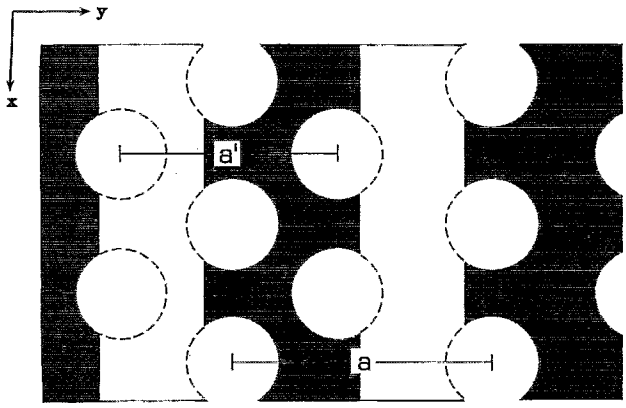

FIG. 6. Plan view in the xy-plane of a structure with misaligned air columns.

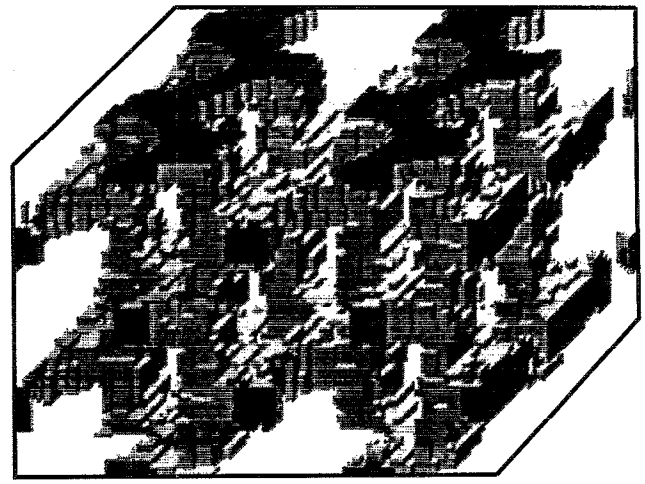

FIG. 7. Three-dimensional photonic crystal structure with overall surface disorder. The disorder is introduced on the interface between the high-index material and air, in the perfect structure shown in Fig. 1.

with misplaced air columns. One specific pattern is shown in Fig. 6. In this pattern, some columns are moved along the y-axis while others are left unchanged. The displacement of the columns is characterized by the parameter a', as shown in Fig. 6. The case of the perfect structure corresponds to $a'=a$. If we let $a'=0.90a$, the gap drops from 23% to 20%.

E. Overall surface roughness

Surface roughness might occur during the growing and etching processes. To address this problem we add a random fluctuation to the surface of every basic dielectric element in the supercell. The average of the disorder is 10% of the dimension of the element and the largest disorder is 20%. The supercell is shown in Fig. 7. The gap for this particular structure is computed to be 19.6%. This basic insensitivity of the photonic band gap to surface roughness arises simply because the mode wavelengths in the vicinity of the gap are much larger than the length scale of the surface disorder.

Finally, since all the types of disorder discussed above may all occur in one structure during the fabrication process, it is interesting to study how their combined presence would influence the size of the gap. For each type of disorder we choose a fluctuation of the same magnitude as discussed earlier, including a misalignment of grooves of 8%, and the parameters of case (a) for both the layer thickness and the groove depth variation. The resulting structure retains a gap of 13.3%. Thus, in general, the photonic band gap appears to be fairly robust in spite of significant surface roughness and element misalignment. As we have shown, the most important effects will arise from deviations that systematically weaken the connectivity of the structure.

ACKNOWLEDGMENTS

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[1] E. Yablonovitch, J. Opt. Soc. Am. B **10**, 283 (1993).
[2] P. R. Villeneuve and M. Piche, Prog. Quantum Electron. **18**, 152 (1994).
[3] K. M. Ho, C. T. Chan, and C. M. Soukoulis, Phys. Rev. Lett. **65**, 3152 (1990).
[4] E. Yablonovitch, T. J. Gmitter, and K. M. Leung, Phys. Rev. Lett. **67**, 2295 (1991).
[5] H. S. Sozuer and J. W. Haus, J. Opt. Soc. Am. B **10**, 296 (1993).
[6] K. M. Ho, C. T. Chan, C. M. Soukoulis, R. Biswas, and M. Sigalas, Solid State Commun. **89**, 413 (1994).
[7] H. S. Sozuer and J. P. Dowling, J. Mod. Opt. **41**, 231 (1994).
[8] S. Fan, P. R. Villeneuve, R. D. Meade, and J. D. Joannopoulos, Appl. Phys. Lett. **65**, 1466 (1994).
[9] H. I. Smith and M. L. Schattenburg, IBM J. Res. Develop. **37**, 319 (1993).
[10] M. C. Peckerar and J. R. Maldonado, Proc. IEEE **81**, 1249 (1993).
[11] R. F. W. Pease, J. Vac. Sci. Technol. B **10**, 278 (1992).
[12] R. D. Meade, A. M. Rappe, K. D. Brommer, J. D. Joannopoulos, and O. L. Alerhand, Phys. Rev. B **48**, 8434 (1993).