The influence of a surface roughness on the transmission properties of 1D photonic crystals.

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Abstract.
In this contribution we present numerical simulations as well as experimental investigations of 1D photonic crystal with intentionally introduced surface roughness. Transmission experiments were performed in the microwave region on a mm-sized structure with roughness of the order of 10 percent. The simulations show the general effect of band edges smearing and reducing of the depths of the gaps. However, the effect becomes significant only for wavelengths which are of the same order with the surface roughness features. Besides, we have shown that if increasing roughness cause decreasing of air filling fraction of a photonic crystal this lead to "shrinking" of the entire band structure resulting in redshift of the gaps edges.

1. Introduction

Photonic crystals (PhC) have been intensively investigated since the beginning of the 1990s when the possibility of the existence of photonic band gaps in periodic dielectric lattices demonstrated first by numerical simulation [1] and then experimentally [2]. During the last years the development of this area is characterized by the tendency to miniaturization of photonic crystals with the main aim to scale down the working range to the near IR and visible regions. It is evident that more and more precise fabrication techniques are required for the realization of this task. Thus, the problem of the influence of disorder on the properties of photonic crystals has attracted a great deal of attention. Since defects and inaccuracies in the determination of the geometrical parameters of real structures are inevitable phenomena in sub-micrometer fabrication, the disorder-induced modifications of photonic crystal properties must be taken into account.

In this publication we present both theoretical and experimental investigations on 1D dielectric photonic crystals with surface roughness. Transmission experiments were performed in the microwave region on a mm-sized structure with roughness of the order of 10 percent. Because of the large dimensions it is possible to design the roughness instead of having to consider it as a fabrication-related feature which is difficult to control. Due to the scalability of Maxwell's equations the main conclusions are valid for down-sized structures like submicron-sized photonic crystals for the near infrared and visible part of the spectrum.

2. Description of the model

In order to simulate the surface roughness the following model was developed. Each high-index dielectric layer of 1D photonic crystal is constructed of narrow bars (Fig. 1). Uniformly distributed random variation of the height of each bar in the direction perpendicular to the interfaces creates the surface roughness. The simulations (in accordance with the PhC in the experiments) were carried out for a five-layer dielectric-air structure with the following parameters: thickness of the dielectric layers is *1.07 mm*, the refractive index is *3.1*, the air spacings between the plates are *1.22 mm* which corresponds to a period of the structure of *a=2.29 mm.* The width of a single bar is 107 μm the total width of each layer is 32 mm.

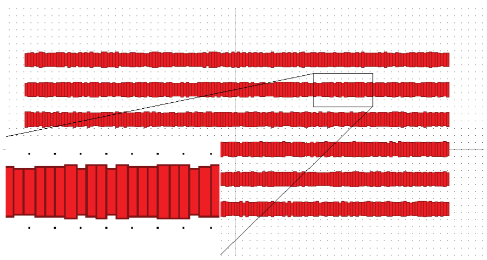

Fig. 1. The model of 1D photonic crystal with surface roughness.

We consider two types of the surface roughness. In

roughness type 1 the mean length of the bars remains the same as in the perfect PC but the individual lengths are multiplied by a random factor: $l_{bar}=l_h(1+\delta_1*P_{-1;1})$ (1); l_{bar} is the perturbed length, l_h is the initial length, $P_{-1;1}$ is a uniformly distributed random value in the range **[-1;1]**, and δ_1 is the roughness amplitude. **Roughness type 2** is given by $l_{bar}=l_h(1+2*\delta_2*P_{0;1})$ (2); all parameters are the same as in type 1 but P is now distributed in the region **[0;1]**. The roughness profiles are different for the different layers. In terms of average thicknesses the total thickness of the PhC is kept constant, i.e. the thickness of the air layer is reduced for type 2.

Ostensibly, the two descriptions yield different results. However, if the type-1 description is applied to a 1D PhC with increased plate thickness $l_h^* = l_h(1+\delta_2)$ (3), the two descriptions are equivalent. The purpose of the two descriptions is to separate different contributions, i.e. the results of the type-1 calculation will be sensitive to details of the surface roughness only whereas those of the type-2 calculations will also reflect the influence of the increase of the average thickness.

The transmission spectra were obtain by FDTD method with perfectly matched layer absorbing boundary conditions in the edges of the computational domain

3. Simulation results

The transmission spectra of 5-layer 1D photonic crystal with type-1 roughness with δ_1=0.4 is shown in Fig. 2a. It is clearly seen from the figure that the surface roughness practically does not affect the lowest band gap. However, the higher the frequency, the higher the effect of the surface roughness. This is easily understandable since the frequency of the center of the first band gap (35 GHz) corresponds to a wavelength $\lambda/n=2.8$ *mm* that is almost *10* times larger than the size of the roughness features. The center of the third band gap (*105 GHz*) corresponds to a wavelength of $\lambda/n=0.94$ *mm* that is already of the order of the roughness. We therefore conclude that the main effect of the roughness type 1 – scattering of the plane wave on surface features – becomes significant when $\lambda / n \sim l_h \cdot \delta_1$, where *n* is the refractive index of the high-index layers.

Fig. 2b shows the transmission spectra for type 2 roughness with δ_2=0.2. It is clearly seen that the band gaps are shifted to the lower frequencies with respect to initial structure. The principal difference between the two roughness descriptions is that for type 2 the length of each bar is larger than in the unperturbed PhC, in other words the air filling fraction is reduced compare to perfect case. This results in "shrinking" of the photonic band structure and, as a consequence, leads to a redshift of the photonic band gaps.

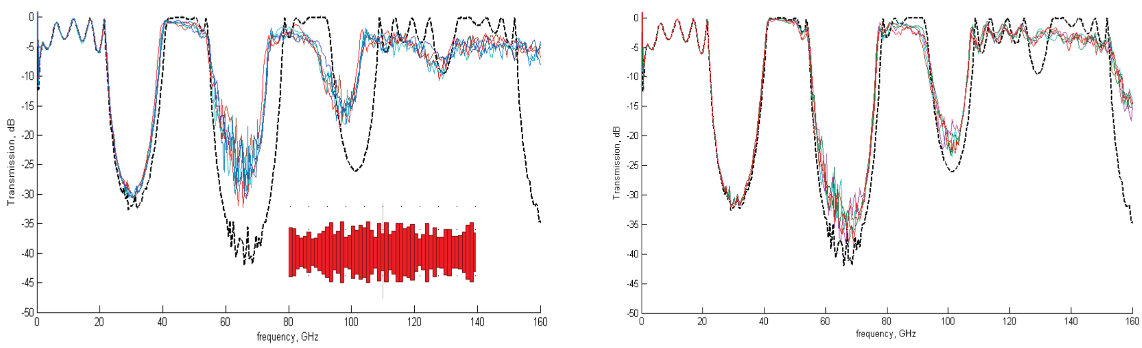

Fig.2. Normal-incidence transmission spectra of 1D 5-layer photonic crystals with surface roughness type 1 with $\delta_1=0.4$ (a) and type 2 with δ_2=0.2 (b). Dashed black line: perfect structure ($l_h=1.07$ μm); dotted blue line: perfect structure with l_h increased to 1.28 μm (in b) only); thin lines of different colors (5 on each plot): different realizations of surface roughness with the same δ. The inset shows a fragment of a high-index layer with δ_1=0.4.

The simplest way to describe this redshift due to reduced air filling fraction is to consider a PhC with zero roughness but with effective thickness of high-index layers recalculated by formula (3) keeping the period unchangeable. The transmission of such structure, showed in Fig. 3b by thick dotted line, fits the transmission curves of disordered PhCs at least up to 60 GHz very good . Actually, if the redshift of the whole spectra is taken into account by formula (3) the effect of roughness type-2 is reduced to type-1. Thus, for type-2 two separate effects contribute: (i) the redshift of the photonic band structure due to the increase of the average thickness of the high-index plates and (ii) the scattering of EM waves at the surface features as for type-1.

4. Experimental transmission

A test sample of a 1D PhC with surface roughness was fabricated. It consists of five alumina plates separated by air with thicknesses given above; the surface roughness was created by gluing alumina powder to both surfaces of each plate. Therefore, the experimental situation is expected to be well described by (2) (type-2). Profilometry measurements showed that the size variation of the alumina powder grains is 30-60 μm.

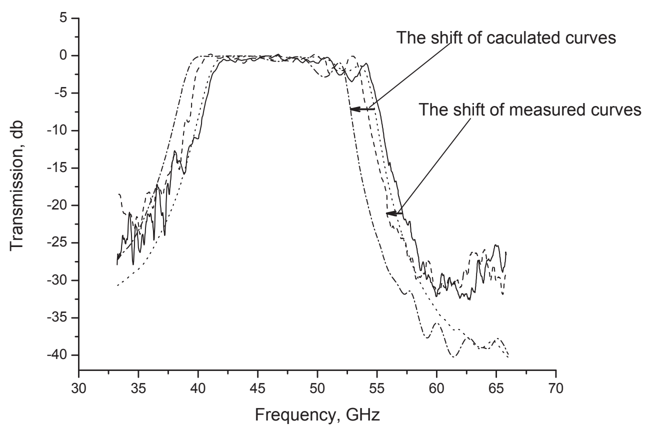

Fig. 3. The transmission spectra in the diapason 33-66 GHz. Solid: measured, zero roughness; dotted: calculated, zero roughness; dashed: measured, PhC with alumina powder; dash dot: calculated, δ2=0.06 that corresponds to maximal height of surface features of 65 μm.

Although in the case of zero roughness the simulated (dotted) curve goes deeper into the band gaps and has steeper gap edge than measured one (solid) the coincidence between the theory and the experiment is good. The surprising result is sufficiently lower redshift of the experimental curve. There are several possible reasons of this discrepancy between the theory and the experiment: (i) uniform random distribution of the roughness features does not reflect the real surface; (ii) the amount of glue (which has a dielectric constant close to 2) on the surface is higher than expected. Profilometry does not distinguish the surface of glue from the surface of smaller grains, optical microscopy gives even less information since only well-reflecting facets of big grains are clearly seen; (iii) the grains have irregular shape thus there might be some spaces filled by air or glue between them.

5. Conclusions

The results of the simulations and the comparison with the experimental data give rise to the following conclusions:

- The effect of surface roughness on the position and width of the lowest band gap is negligible if the average thickness is equal to the thickness of a perfect PhC. Due to the scalability of Maxwell equations we can extend our results to submicron-sized 1D photonic crystals and state that the lowest gap remains unchangeable for any reasonable amount of fabrication imperfections.
- Experiment clearly show the redshift of transmission curves due to increased average thickness of high-index layers, however the amount of this shift is lower than predicted by theory probably due to insufficient characterization of the surface.
- The effect of disorder gets stronger at shorter wavelengths and become significant when $\lambda / n \sim l_h \cdot \delta_1$, where n is the refractive index of the high-index layers, l_h is the thickness of the high-index layers and δ_1 is the amplitude of the surface roughness

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[1] Ho K. M., Chan C. T., Soukoulis C. M., Phys. Rev. Lett. **65,** 3152 (1990); Shang Z., Satpathy S., Phys Rev. Lett. **65**, 2650 (1990); Ho K. M., Chan C. T., Soukoulis C. M., Phys Rev. Lett. **65,** 3152 (1990)
[2] S.L. McCall, P.M. Platzman, Phys. Rev. Lett. **67,** 2017 (1991); Yablonovich E., Gmitter T. J., Leung K. M., **67**, 2295 (1991)