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Calculation of the one-dimensional photonic crystals based on diamond

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Abstract. A model of a one-dimensional photonic crystal based on diamond has been created and its reflectivity has been calculated. The obtained results of the finite element method calculation are compared with preliminary analytical calculations.
Keywords: diamond, photonic crystal, Bragg's reflector, optical resonator, finite element method.

1. Introduction

Due to its unique physical and chemical properties, including: due to its high refractive index, high chemical and radiation resistance, diamond is a promising material for use in various photonic and optical devices [1]. Despite the fact that the presence of impurities, for example, nitrogen, does not have a strong effect on the refractive index of diamond, it still changes by ~1%, which makes it possible to use a structure consisting of a set of diamond layers with and without nitrogen as a photonic crystal [2].

A one-dimensional photonic crystal is a structure with variable alternation of the refractive index in it in one direction [3]. In this case, these are alternating layers of pure diamond and layers of diamond doped with nitrogen. The main advantage of such structures is the possibility of achieving almost one hundred percent reflection in the optical spectrum range of interest. This property makes one-dimensional photonic crystals advantageous for use as laser optical resonators [4].

The purpose of this work is to calculate the reflection spectrum of a one-dimensional photonic crystal for the wavelength range $\Delta\lambda$ = 450–650 nm with a maximum at the wavelength λ = 532 nm.

2. Calculation of reflection spectra

2.1. Preliminary calculation of reflection efficiency

The following formula was used for a preliminary assessment of the efficiency of reflection:

$$R = \left(\frac{1 - \left(\frac{n_h}{n_l}\right)^{2N} \left(\frac{{n_h}^2}{n_a \cdot n_s}\right)}{1 + \left(\frac{n_h}{n_l}\right)^{2N} \left(\frac{{n_h}^2}{n_a \cdot n_s}\right)} \right)^2 , \tag{1}$$

where R – reflection coefficient, n_h – largest refractive index of layer, n_l – smallest refractive index of layer, n_a – refractive index of the medium, n_s – refractive index of the substrate (on which the photonic crystal is deposited), N – number of pairs of layers.

Expression (1) allows us to evaluate the efficiency of reflection, without taking into account the wavelength of the radiation used and the angle of incidence. Based on it, it is obvious that the greater the difference between the refractive indices of the layers, the greater the reflection coefficient is achieved when using the same number of layers.

Table 1 shows the results of calculating the maximum possible reflection coefficient when using different combinations of refractive indices and different number of pairs of layers, where n_h is the refractive index of a pure diamond layer, n_l is the refractive index of a nitrogen-doped diamond layer.

Since the refractive index values of nitrogen-doped diamond n = 2.32 and 2.36 are impossible to obtain, all subsequent calculations were performed for the most realistic combination of refractive indices: $n_h = 2.42$, $n_l = 2.40$. It is also shown here that better reflectance can be obtained with higher contrast and number of layers in the structure.

Table 1. Calculation of reflection coefficient

	Refractive indices n_h - n_l			**Number of pairs of layers N**
	2.42 - 2.32	2.42 - 2.36	2.42 - 2.40	
The maximum possible reflection coefficient R, %	48.8	36	23.2	10
	73.6	54.3	29.4	20
	97.6	87.4	48.2	50
	100	98.9	73	100
	100	100	94.2	200

2.2. Finite element method calculation

In this paper, the finite element method was used to calculate the parameters of a diamond-based one-dimensional photonic crystal, including calculation of the values of the maximum possible reflection.

To determine the thickness of the layers in the calculated one-dimensional photonic crystal, the derivation from the Wolf-Bragg condition was used:

$$d = \frac{m\lambda}{4n \cdot \sin\theta}, \qquad (2)$$

where d – thickness of one layer, λ – wavelength of incident radiation, θ – angle of incidence of radiation to the surface, n – refractive index of the layer, m – integer.

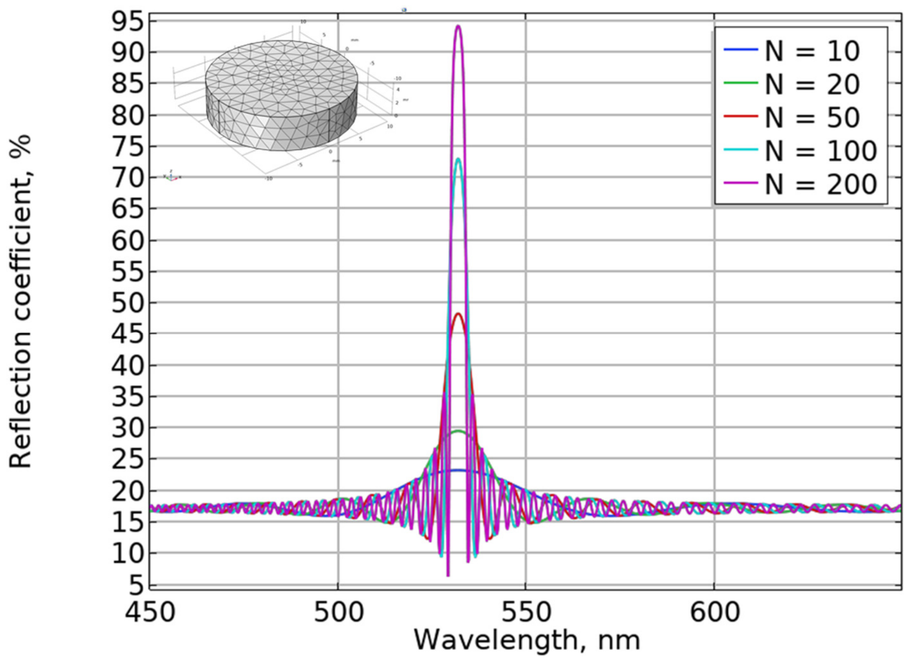

Fig.1 Calculated reflection spectra for diamond photonic crystal set at 532 nm.

According to formula (2), the thickness of each layer directly depends on the number of wavelengths that fit into one period of a one-dimensional photonic crystal, and on the angle of incidence. Each layer in this structure can be defined as a quarter-wave plate.

Due to the possible use of the calculated structure as mirrors of an optical resonator, all calculations were carried out for the wavelength of the exciting laser of interest $\lambda = 532$ nm and normal fall. To get the most realistic results, two models were created: the transmission model and the reflection model.

Fig.1 shows the calculated reflection model of a one-dimensional photonic crystal constructed in the COMSOL Multiphysics. The geometry of this model is a single cylinder with the specified parameters; this cylinder is a diamond substrate on which a one-dimensional photonic crystal is applied. This model was created in COMSOL “Geometric optics” module which means that this is simplified model of the photonic crystal and there is no way to set refractive indices of layers as table.

Fig.2 shows the calculated transmission model of a one-dimensional photonic crystal constructed in the COMSOL Multiphysics. The geometry of this model is 2D rectangle with a number of layers on it. This model was created in COMSOL “Wave optics” module which means that this is more suitable model of the photonic crystal and if necessary, some material properties can be set for each layer.

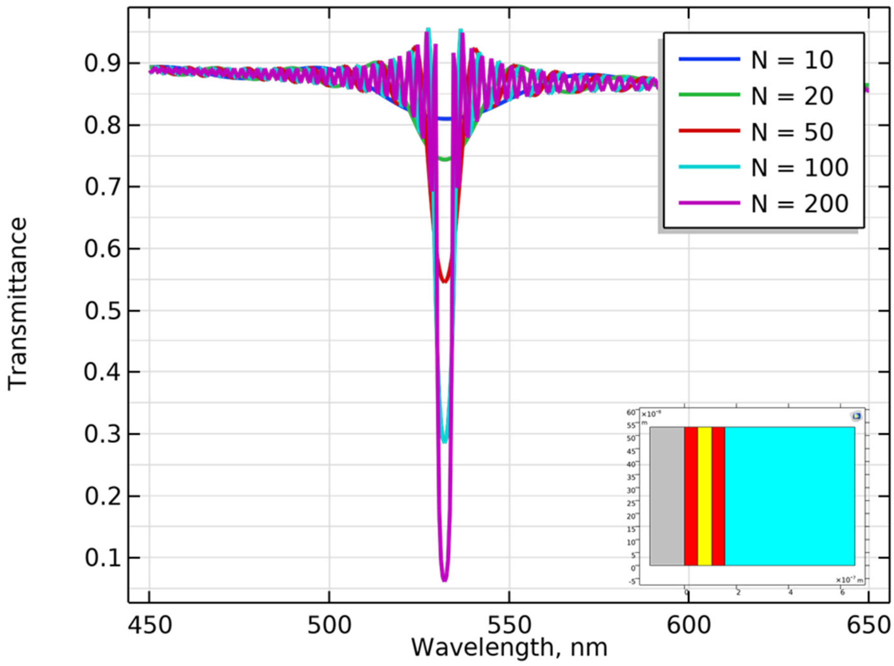

Fig. 2 Calculated transmission spectra for diamond photonic crystal set at 532 nm.

It is shown that with an increase in the number of pairs of layers used, the maximum achievable reflection coefficient increases, however, when a certain number of pairs of layers is reached, this indicator will reach 100% and, accordingly, will stop growing. During the calculation, it was found that the number of pairs of layers $N = 200$ is the optimal value.

3. Conclusion

A preliminary assessment and subsequent calculation of the reflection spectrum of a one-dimensional photonic crystal based on diamond was carried out. It is established that, when using successively alternating layers of pure diamond and nitrogen-doped diamond, it is possible to create a structure that does not allow radiation of a given wavelength to pass through it. When using a different number of pairs of layers, a different result is achieved.

So, when using 200 pairs of layers, it is possible to achieve a reflection coefficient of $R = 94\%$, which allows using this structure as a blind mirror for a resonator. At the same time, using 50 pairs of layers, the achievable reflection coefficient is $R = 48\%$, which allows you to create a translucent mirror.

Thus, it becomes possible to create an optical resonator tuned to the wavelength of the exciting laser λ = 532 nm, so that the exciting radiation will make several passes through the active medium of the diamond laser and increase its gain.

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5. References

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