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Simplified Bragg–Snell law applicability for anodic alumina oxide photonic crystals

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In this research we show the results of the simplified and general Bragg–Snell law comparison in determination of photonic band gap position. Aforementioned law is used for describing anodic aluminum photonic crystals. The results were obtained by varying different parameters in calculations.

Keywords: photonic crystal, aluminum oxide, porous material, photonic band gap, anodizing, effective refractive index.

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A photonic crystal (PC) is a solid body that is basically a periodic spatial structure with a varying permittivity and a characteristic structural element size on the order of the optical wavelength. The simplest example of a PC is a structure consisting of two alternating types of parallel optical layers, each of which has its own permittivity and thickness. The main feature of a PC, which manifests itself in interaction with electromagnetic radiation, is the emergence of band gaps (spectral regions where radiation is reflected partially or completely by the crystal in one or all directions due to constructive interference). The interest in such structures stems primarily from their applicability as manipulators and collectors of light energy [1,2].

One of the simplest yet most promising ways to synthesize PCs is the anodic treatment of metal foil. The main materials used in this type of crystal synthesis are titanium and aluminum. Aluminum foil turned out to be the best suited for this process: anodic aluminum oxide (AAO) Al_2O_3 PCs [3] are grown readily on its surface. One may adjust the porosity of AAO and the shape of the pores, which have a direct effect on the optical properties of a PC, by changing the anodic treatment conditions. Notably, aluminum oxide is a dielectric material with a low coefficient of light absorption within the visible and near infrared ranges [4]. Periodic structures with the indicated properties have wide application opportunities as, e. g., optical filters, sensors, etc. [5–9].

The Bragg–Snell, which also called simply Bragg's law, allows one to find the angles and wavelengths corresponding to reflection maxima or transmission minima. The following simplified version of it is used in certain studies [8–11] focused on AAO PCs:

$$m\lambda = 2d\sqrt{n_{eff}^2 - n_A^2 \sin^2\varphi}, \qquad (1)$$

where λ is the center wavelength of the band gap, m is the band gap order, d is the structure period, φ is the light incidence angle, n_{eff} is the effective refraction index of a crystal, and n_A is the refraction index of the ambient medium.

It has been established empirically that formula (1) provides a highly accurate estimate of the band gap position in AAO PCs. However, this is not true for other materials. Although relation (1) is often used to characterize the properties of AAO PCs, we are not aware of any studies where the conditions of applicability of this formula to these media are discussed. The present paper should fill this gap and is aimed at determining numerically the applicability domain of relation (1).

Let us consider the propagation of light within a structure consisting of two alternating types of parallel optical layers. We denote the band gap wavelength corresponding to order m, where m is a positive integer, as λ; the thicknesses of layers with refraction indices n_1, n_2 as d_1, d_2, respectively; the refraction index of the ambient medium as n_A; and the angle of incidence of an electromagnetic wave on the layered structure, which is measured from the normal to the surface, as φ. Figure 1 shows the path of two rays within such a structure. The optical path length of a ray reflected from deeper layers of a crystal is

$$L = 2(d_1 n_1 \cos\theta_1 + d_2 n_2 \cos\theta_2). \qquad (2)$$

Using Snell's law, we find the equations relating φ, θ_1, θ_2:

$$\sin\theta_1 = \frac{n_A}{n_1}\sin\varphi,$$

$$\sin\theta_2 = \frac{n_1}{n_2}\sin\theta_1 = \frac{n_A}{n_2}\sin\varphi. \qquad (3)$$

The condition of interference maximum of two reflected rays then takes the form

$$L = d_1\sqrt{n_1^2 - n_A^2\sin^2\varphi} + d_2\sqrt{n_2^2 - n_A^2\sin^2\varphi} = \frac{\lambda}{2}m. \qquad (4)$$

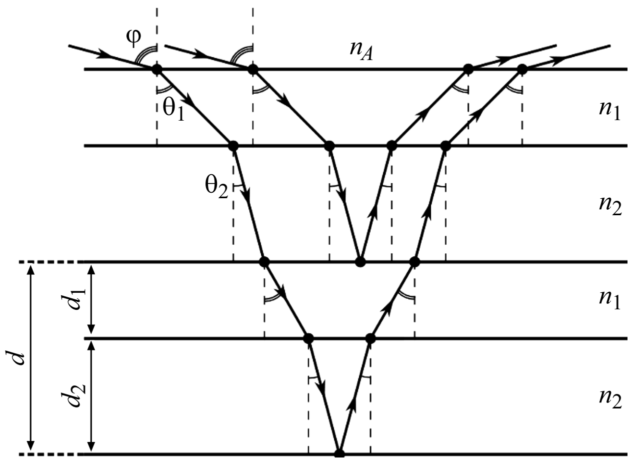

Figure 1. Path of rays within a structure consisting of two alternating types of parallel optical layers.

The resulting expression is the well-known Bragg–Snell law [12].

If n_1 and n_2 are similar in value, relation (1) may be derived by algebraic transformations from Eq. (4). This approximation is typical for synthesized AAO PCs. The effective refraction index of a crystal may be determined in the following manner:

$$n_{eff}^2 = \frac{d_1}{d_1 + d_2} n_1^2 + \frac{d_2}{d_1 + d_2} n_2^2. \quad (5)$$

If one substitutes n_1 with n_2 or n_2 with n_1 (on the assumption that $n_1 \approx n_2$) in expression (5), equality $n_1 \approx n_2 \approx n_{eff}$ is obtained. Substituting n_1 and n_2 in (4) with n_{eff}, we find expression (1).

The domain of applicability of relation (1) may be found by direct comparison with formula (4). Let us examine the dependence of error $\Delta\lambda/\lambda_1$ on n_2/n_1 (Fig. 2), where $\Delta\lambda = |\lambda_1 - \lambda_2|$, λ_1 is calculated using formula (4), λ_2 is calculated using formula (1), and n_1 and n_2 are the refraction indices of PC layers. The parameters of one of the layers are fixed: $n_1 = 1.2$, $d_1 = 150$ nm (Fig. 2, *a*); $n_1 = 1.2$, $d_1 = 450$ nm (Fig. 2, *b*); $n_1 = 1.5$, $d_1 = 150$ nm (Fig. 2, *c*); and $n_1 = 1.5$, $d_1 = 450$ nm (Fig. 2, *d*). Parameters d_2, n_2 of the other layer and the angle of incidence of radiation on the PC, which is measured from the normal to the surface, vary.

The obtained dependences (Fig. 2) correspond to the variation of two parameters of the second layer: thickness d_2 and refraction index n_2, which assume values characteristic of the synthesized PCs. This provides an opportunity to compare the influence of the layer thickness (refraction index) with a certain refraction index (layer thickness) being fixed on the final error value.

A significant influence of radiation incidence angle φ on the rate of error growth is typical of all values of thickness parameters and refraction indices of layers. The error increases with increasing angle. This growth is most pronounced when n_2 tends to unity, which is typical of crystals with a high porosity [5].

Figure 2, *c* corresponds to a small layer thickness and a relatively high refraction index. Comparing it with Fig. 2, *d* (larger layer thickness), one sees clearly that the error derivative increases in absolute value as the layer becomes thicker. It follows from a comparison of Fig. 2, *c* with Fig. 2, *a* (lower refraction index) that the error derivative increases in absolute value as the refraction index decreases. Figure 2, *b*, which corresponds to a large layer thickness and a low refraction index, demonstrates the highest absolute value of the error derivative among all the plots presented.

Let us determine the specific values of error at $\varphi = 0$. The maximum error is observed at the plot points corresponding to n_2 values tending either to 1 or to ∞. In the former case, the error assumes the following values:

Fig. 2, *a* — $\Delta\lambda/\lambda_1(1/1.2) \approx 0.3\,\%$,
Fig. 2, *b* — $\Delta\lambda/\lambda_1(1/1.2) \approx 0.4\,\%$,
Fig. 2, *c* — $\Delta\lambda/\lambda_1(1/1.5) \approx 1.8\,\%$, and
Fig. 2, *d* — $\Delta\lambda/\lambda_1(1/1.5) \approx 1.6\,\%$.

It is definitely pointless to examine the latter case, since it is inconsistent with the problem at hand; however, the error is quite significant already at $n_2 = 2n_1$:

Fig. 2, *a* — $\Delta\lambda/\lambda_1(2) \approx 3\,\%$,
Fig. 2, *b* — $\Delta\lambda/\lambda_1(1) \approx 5.4\,\%$,
Fig. 2, *c* — $\Delta\lambda/\lambda_1(2) \approx 3\,\%$, and
Fig. 2, *d* — $\Delta\lambda/\lambda_1(2) \approx 5.4\,\%$.

As was already noted, the error increases at large angles φ.

The refraction index of a single crystal of aluminum oxide at a wavelength of 555 nm is 1.63 [4]. It follows from Fig. 2 that the error for the limit PC value of $n_2 = 1.63$ at $\theta = 0$ is:

Fig. 2, *a* — $\Delta\lambda/\lambda_1(1/n_1) \approx 1.3\,\%$,
Fig. 2, *b* — $\Delta\lambda/\lambda_1(1/n_1) \approx 1.85\,\%$,
Fig. 2, *c* — $\Delta\lambda/\lambda_1(1/n_1) \approx 0.25\,\%$, and
Fig. 2, *d* — $\Delta\lambda/\lambda_1(1/n_1) \approx 0.33\,\%$.

Thus, the error associated with the use of formula (1) is insignificant in the case of AAO PCs.

The position of the band gap of a one-dimensional PC is characterized by the Bragg–Snell law. A simplified approximate formula is commonly used to determine the PC properties, but its applicability domain remained undefined. The error introduced by the simplified formula was determined numerically. Its application to real AAO PCs is fully justified, since the error introduced is extremely small.

With normal incidence of radiation on a PC, the actual error associated with formula (1) will not exceed 2 %. In the case of large incidence angles, the error may become significant (6 %) if the refraction indices of PC layers are small (≤ 1.2) or differ widely from one layer to the other.

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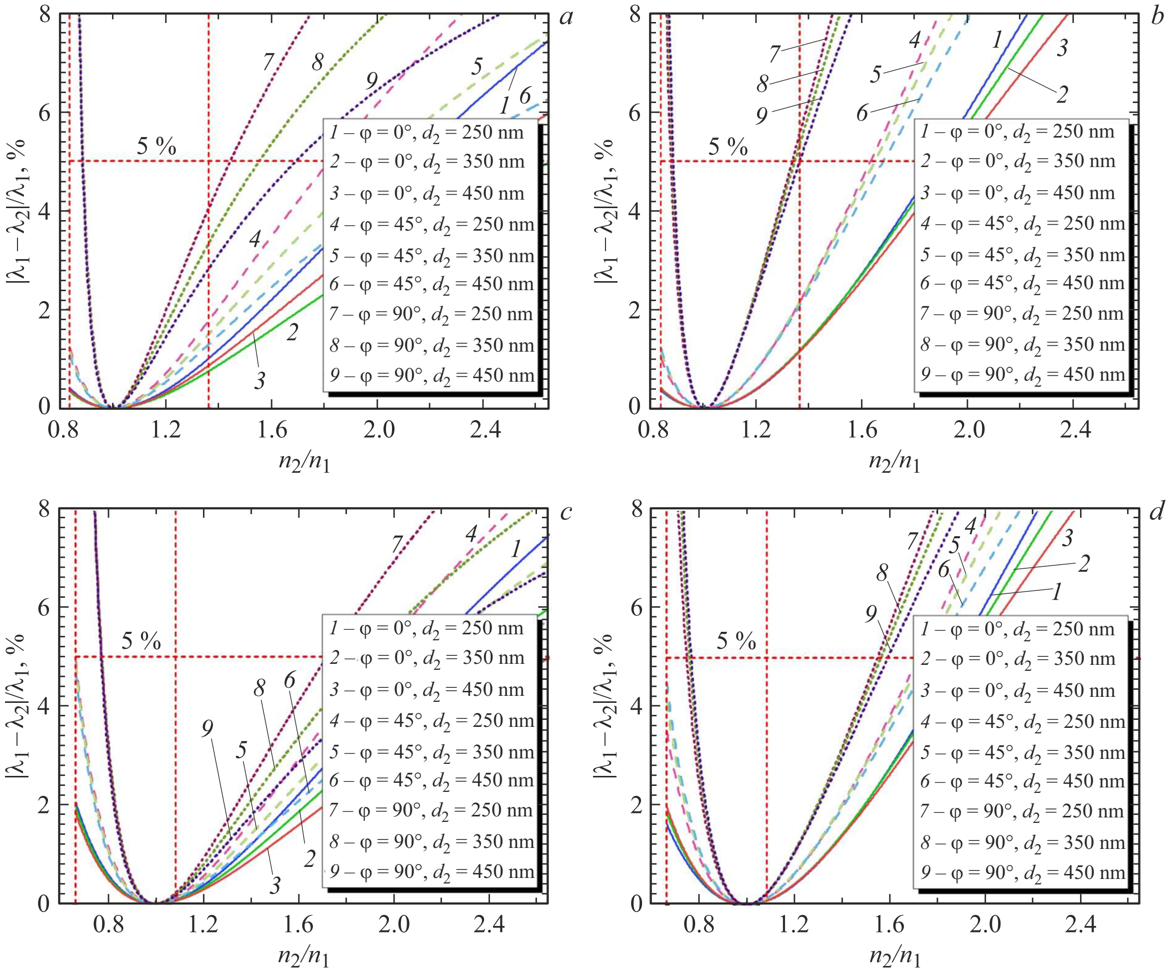

Figure 2. Deviations of the band gap position at different PC parameters. *a* — $d_1 = 150$ nm, $n_1 = 1.2$; *b* — $d_1 = 450$ nm, $n_1 = 1.2$; *c* — $d_1 = 150$ nm, $n_1 = 1.5$; *d* — $d_1 = 450$ nm, $n_1 = 1.5$. Vertical dashed lines correspond to $n_2 \to 1$ (left) and $n_2 = n_{Al_2O_3} = 1.63$ (right).

Conflict of interest

The authors declare that they have no conflict of interest.

References

[1] B.E.A. Saleh, M.C. Teich, *Fundamentals of photonics* (John Wiley and Sons Inc., Hoboken, 2007).

[2] I.A. Sukhoivanov, I.V. Guryev, *Photonic crystals: physics and practical modeling*. Springer Ser. in Optical Sciences (Springer, Berlin–Heidelberg, 2009), vol. 152. DOI: 10.1007/978-3-642-02646-1

[3] G. Shang, D. Bi, V.S. Gorelik, G. Fei, L. Zhang, Mater. Today Commun., **34**, 105052 (2023). DOI: 10.1016/j.mtcomm.2022.105052

[4] W.J. Tropf, M.E. Thomas, *Handbook of optical constants of solids* (Academic Press, 1997).

[5] C.S. Law, S.Y. Lim, A.D. Abell, N.H. Voelcker, A. Santos, Nanomaterials, **8** (10), 788 (2018). DOI: 10.3390/nano8100788

[6] I.A. Kalinin, I.V. Roslyakov, D. Bograchev, S.E. Kushnir, I.I. Ivanov, A.V. Dyakov, K.S. Napolskii, Sensors Actuators B, **404**, 135270 (2024). DOI: 10.1016/j.snb.2023.135270

[7] A.R. Gómez, L.K. Acosta, J. Ferré-Borrull, A. Santos, LF. Marsal, ACS Appl. Nano Mater., **6** (7), 5274 (2023). DOI: 10.1021/acsanm.2c05356

[8] S.E. Kushnir, K.S. Napolskii, Mater. Des., **144**, 140 (2018). DOI: 10.1016/j.matdes.2018.02.012

[9] M.V. Pyatnov, M.M. Sokolov, I.A. Kiselev, R.G. Bikbaev, P.S. Pankin, I.R. Volkova, V.A. Gunyakov, M.N. Volochaev, I.I. Ryzhkov, S.Ya. Vetrov, I.V. Timofeev, V.F. Shabanov, Tech. Phys., **69** (2), 265 (2024).

[10] V.S. Gorelik, M.M. Yashin, D. Bi, G.T. Fei, Opt. Spectrosc., **124** (2), 167 (2018). DOI: 10.1134/S0030400X18020078.

[11] P.P. Sverbil, V.S. Gorelik, D. Bi, G.T. Fei, S.H. Xu, X.D. Gao, Opt. Spectrosc., **127** (4), 602 (2019). DOI: 10.1134/S0030400X1910028X.

[12] A. Yariv, P. Yeh, *Optical waves in crystals* (Wiley, N.Y., 1984).

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