УДК 535.3, 535.5

СВЕТОПОГЛОЩАЮЩАЯ СПОСОБНОСТЬ ГИПЕРКРИСТАЛЛОВ

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Аннотация. Использована теория электромагнитных волн в немагнитных многослойных гиперкристаллах, определены их спектральные свойства и записаны дисперсионные соотношения для обыкновенной и необыкновенной волн. Показано, что отражение волн от гиперкристалла подавляется, в то время как поглощение волн в гиперкристалле возрастает, если его волновой импеданс согласован с импедансом окружающей среды. При изучении поглощательных свойств гиперкристаллов обращается внимание на зависимость поглощения от толщин входящих в гиперкристалл слоев. Получено, что пик спектра поглощения растет с увеличением толщины разделительного диэлектрического слоя и смещается в область длинных волн. Установлено, что зависимость поглощения от доли металла в структуре задается дисперсионными свойствами гиперкристаллов (более низкое поглощение отмечено для больших долей металла). Величины пика поглощения и ширины зоны поглощения могут меняться в зависимости от числа слоев, достигая требуемых значений. Результаты настоящего исследования найдут применение в нанофотонике и физике солнечных элементов для широкополосного увеличения поглощения электромагнитного излучения.

Ключевые слова: электромагнитная волна; гиперболический метаматериал; гиперкристалл; поглощение; импеданс.

Благодарность. Работа выполнена при финансовой поддержке Министерства образования Республики Беларусь (задание 2.2.3 государственной программы научных исследований «Фотоника и электроника для инноваций» на 2021–2025 гг., № гос. регистрации 20211793).

Образец цитирования:
Сюй Ч, Новицкий АВ. Светопоглощающая способность гиперкристаллов. *Журнал Белорусского государственного университета. Физика.* 2024;2:4–10 (на англ.).
EDN: UCLOCM

For citation:
Xu Ch, Novitsky AV. Light absorption abilities of hypercrystals. *Journal of the Belarusian State University. Physics.* 2024; 2:4–10.
EDN: UCLOCM

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LIGHT ABSORPTION ABILITIES OF HYPERCRYSTALS

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Abstract. Here, we employ the theory of electromagnetic waves in non-magnetic multilayer hypercrystals to determine their spectra and derive dispersion relations for ordinary and extraordinary waves. We demonstrate that the reflection of a hypercrystal vanishes, while the absorption increases, if its wave impedance is matched to that of the surrounding medium. We study the absorption properties of hypercrystals focusing on absorption dependence on thicknesses of available layers. We reveal that the peak values of absorption increase for thicker spacer layer, while the wavelength at the peak is red-shifted. Dependence on the filling fraction of metal is shown to be strongly dependent on the dispersive properties of hypercrystals exhibiting lower absorption for greater filling fractions, while the absorption peak value and absorption bandwidth can be tailored with number of layers. This research might be useful for maximsing absorption to achieve a broadband perfect absorber on the hypercrystal platform.

Keywords: electromagnetic wave; hyperbolic metamaterial; hypercrystal; absorption; impedance.

Acknowledgements. The research was supported by the Ministry of Education of the Republic of Belarus (assignment 2.2.3 of the state programme of scientific research «Photonics and electronics for innovations», 2021–2025; state registration No. 20211793).

Introduction

Hypercrystals [1] have attracted attention in recent years due to their extraordinary properties prospective for the development of novel optical devices. One of the key challenges of hypercrystals is improving their absorption capabilities owing to capturing and utilisation of the incident light. By optimising the absorption characteristics of hypercrystals, researchers aim to maximise their performance in applications such as photovoltaics, photocatalysis, and photodetection. Several approaches have been proposed to enhance absorption in hypercrystals.

The first approach is based on the design and engineering of the hypercrystal structure at the nanoscale by tailoring the geometrical dimensions (size and shape) and the sequence of the involved elements. Plasmonic nanoparticles embedded in a hypercrystal is a good example of light absorption enhancement technique caused by the localised surface plasmon resonance. Another strategy exploits light trapping in hypercrystals due to the confinement and multiple scattering of light in the photonic structure. The multiple scattering increases absorption by means of the elongation of the optical path length, being realised using surface texturing, photonic crystals and waveguides. Light-absorbing materials and dyes incorporated into hypercrystals are a straightforward mean of absorption enhancement. Organic or inorganic chromophores widen the absorption spectral range of hypercrystals. The abovementioned approaches are very useful for applications as multispectral imaging and solar energy harvesting. Below we give recent references on the light absorption in hypercrystals. In the work [2] was employed plasmonic nanoparticles to raise light absorption and short circuit current density of GaAs solar cells. Authors in the work [3] employed a hyperbolic metamaterial nanoparticle structure to form structured surfaces with near-perfect absorption properties. Magneto-optical hypercrystals proposed in [4] can serve as a unidirectional light absorber operating in a wide range of angles.

This paper examines hypercrystals composed of alternating dielectric layers and hyperbolic metamaterials (HMMs) [5–7]. The paper focuses on the first approach mentioned above, which involves varying the dimensional and structural properties of hypercrystals to achieve enhanced absorption. The aim is to achieve a wider range of optical modulation over a wider range of optical wavelengths, as well as improved light absorption. The research is conducted for normally incident visible light. The study is focused on impedance matching of waves in the hypercrystal and those in an ambient medium to facilitate reflection reduction and, consequently, enhance absorption. The stack of layers is altered to achieve as great absorbance as possible.

Description of waves in hypercrystals

Figure 1 shows the structure of a hypercrystal [1] comprising a periodical array of two layers, which are the hyperbolic and natural media. The hyperbolic metamaterial achieves its special properties due to the composition of alternating silver metal (A) and silicon dielectric (B) layers. A natural medium (C) or, in other words, a spacer is either air or glass. By varying the structural properties of the hypercrystals we aim at reaching as much hypercrystal's absorbance as possible. Here we consider the hypercrystal as stack of layers $((AB)_{10}C)_7$. The lower index shows, how many periods we take, e. g., $(AB)_{10}$ means 10 periods of layers A and B. The period of the hypercrystal is much smaller than the free-space wavelength as $d \ll \lambda_0$, but well above the unit cell size of the hyperbolic metamaterial $d \gg a$.

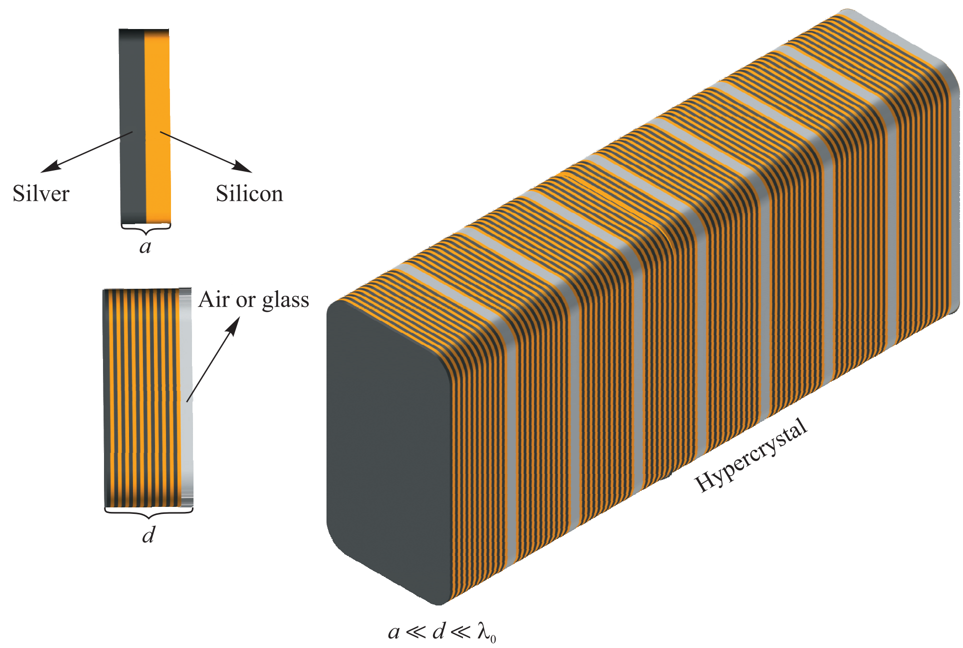

Fig. 1. Structure of the hypercrystal as a periodic variation of the composite hyperbolic and dielectric media

Electromagnetic wave propagation is a hypercrystal can be described as follows. At first, we solve the Maxwell equations in each homogeneous slab with its own isotropic dielectric permittivity ε and magnetic permeability $\mu = 1$. We take the plane of incidence to be the plane XZ and the axis Z is the direction of stratification [8] as shown in fig. 2, where $\mathbf{k}_i$ is the wave vector of the incident wave and $\mathbf{k}_x = b\mathbf{e}_x$ is the component of the wave vector along the axis X. Then we use the boundary conditions to determine the reflection and transmission coefficients. Generally speaking, the theory of waves in multilayer systems [9–11] is involved for finding characteristics of reflected and transmitted electromagnetic waves in multilayer hypercrystals.

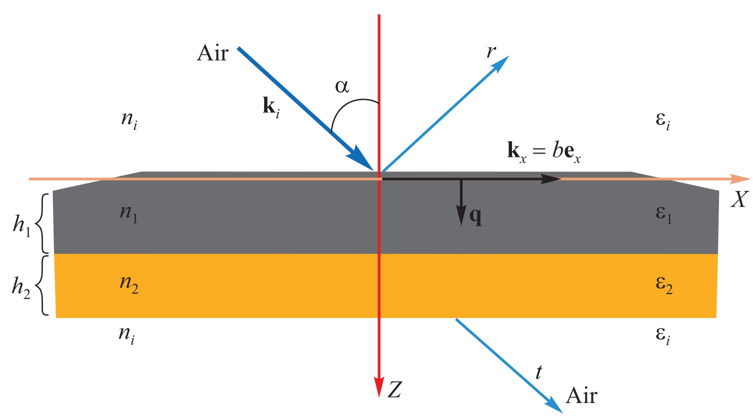

Fig. 2. Schematic of the wave reflection and transmission

Absorption properties of hypercrystals

Dispersion of a hypercrystal. Dispersion causes light waves of different wavelengths to propagate at different speeds in hypercrystals, which can affect the phase and amplitude of the light waves, and therefore the absorption properties of the hypercrystals. Dispersion can be defined as dependence of the wavevector on the frequency, the real and imaginary parts of which govern the phase and the amplitude, respectively.

Photonic hypercrystal comprises alternating layers of air and hyperbolic metamaterial, the latter being composed of alternating metal layers and dielectric layers. Considering silver metal layer and silicon dielectric layer as constituents of the hyperbolic metamaterial and an air layer as a dielectric spacer, one can get a spherical and ellipsoidal refractive surfaces corresponding to respectively ordinary and extraordinary waves in the hypercrystal as an effective uniaxial crystal.

So, let us discuss how the dispersive properties of photonic hypercrystals may affect its absorptivity. Light waves of various wavelengths have different speeds in the hypercrystal, thus, resulting in different interaction times with the composite material and causing a spectral shift in the position of an absorption peak. The dispersion also influences the intensity of light absorption in the hypercrystal exhibiting its wavelength dependence. When resonance conditions in the hypercrystal are met, the dispersion can cause the propagation of light waves to align with the absorption peaks of the material, resulting in increased absorption at those wavelengths.

Impedance matching of a hypercrystal. In this subsection, we calculate the absorption spectrum of the hypercrystal in conditions of impedance matching that is assumed to increase the absorptivity of the hypercrystal. We consider the wave incidence from an air to the hypercrystal and the impedance matching means that the impedance of the hypercrystal coincides with that of the surrounding air. With the impedance matching, the reflected intensity is strongly suppressed. At the same time, the absorptivity may increase up to 1, if the transmissivity is about zero due to a highly reflective substrate behind [12; 13].

The hyperbolic medium is composed of a 3 nm metal layer and a 6 nm dielectric layer with a permittivity of 1. Hypercrystal has a periodic stacked structure $((AB)_{10}C)_{45}$.

To determine the impedance, the retrieval technique developed in [14] can be used. The retrieval procedure implies finding refractive index n and wave impedance z (or dielectric permittivity $\varepsilon = \frac{n}{z}$ and magnetic permeability $\mu = nz$) basing on the reflection and transmission spectra.

A scattering matrix (S) relates the incoming field amplitudes to the outgoing field amplitudes, and can be directly related to experimentally determined quantities [14]. The elements of the matrix S can be found using the elements of the transfer matrix and eventually read as

$$S_{21} = S_{12} = \frac{1}{\cos(nkd) - \frac{i}{2}\left(z + \frac{1}{z}\right)\sin(nkd)} \tag{1}$$

and

$$S_{11} = S_{22} = \frac{i}{2}\left(\frac{1}{z} - z\right)\sin(nkd). \tag{2}$$

Equations (1) and (2) can be inverted to find the wave impedance in terms of the scattering parameters as [14]

$$z = \sqrt{\frac{(1 + S_{11})^2 - S_{21}^2}{(1 - S_{11})^2 - S_{21}^2}}. \tag{3}$$

Thus, determining the matrix S elements $S_{11} = r$ and $S_{21} = t\exp(ik_0 d)$ from the transfer-matrix approach, we can calculate the impedance. We can notice that in reflectionless conditions the impedance equals unity. And vice versa, if the impedance $z = 1$, then the reflection vanishes.

Real part of the impedance computed according to equation (3) is depicted in fig. 3, *a*. The impedance is close to 1 (the impedance of the ambient medium) at an incident wavelength of 643 nm, which well corresponds to the wavelength of absorption peak shown in fig. 3, *b*, the absorption being calculated as $A = 1 - |S_{11}|^2 - |S_{21}|^2$. The impedance matching does not guarantee the perfect absorption $A = 1$ due to the wave transmission through the hypercrystal. However, if the transmission can be eliminated, for instance, using a mirror right after the hypercrystal, then one can expect the perfect absorption at the wavelength of the impedance matching.

Maximisation of absorption for stacked structure $((AB)_{10}C)_7$. Figure 4 demonstrates close absorptivity of the HMM and the hypercrystal achieved for the 10 nm thick air spacer and the 9 nm thick HMM unit cell. Both have a peak absorptivity of approximately 0.699 at the wavelengths near 493 nm. Two structures have almost identical absorption properties. However, what happens if the thickness of the anisotropic layer is increased or decreased?

Variation of the absorption spectral peak is illustrated in fig. 5 for the hypercrystal periodic structure $((AB)_{10}C)_7$. The thicknesses of the metal and dielectric layers in the HMM unit cell of thickness a are equal to a_m and a_d, respectively. Filling fraction of the metal is defined as $f = \frac{a_m}{a_m + a_d}$. To specify the unit cell, we can use either thicknesses of layers a_m and a_d or the thickness of the cell and the filling fraction as in fig. 5. From fig. 5, *a*, we know, how the absorption peak behaves depending on the structure of the HMM unit cell and the spacer thickness, that is, on the geometry of the hypercrystal unit cell. The number of points in fig. 5 is limited with the condition $\frac{\lambda}{d} > 7$. The maximum absorption 0.73 is achieved in this case. For the fixed filling fraction, the absorption increases, if the thickness of the unit cell increases. It is an obvious consequence of the growth or the amount of metal. However, the dependence on the filling fraction or the thickness of the spacer is more complex owing to the dispersive properties of the hypercrystal. We observe that although the amount of metal decreases, the absorption raises. According to fig. 5, *b*, the wavelength at the absorption peak has a clear red shift upon increasing the HMM unit cell at $f = 0.5$, but floats for $f = 0.3$. The dependence on the air spacer thickness is near linear showing a red shift of the absorption maximum. Figure 5, *c*, demonstrates the absorption peak characteristics in one graph. Lower values of filling fraction result in greater absorption owing to the stronger localisation of the electromagnetic field in the metal.

In fig. 5, *d*, one can see the absorption – wavelength diagram for a glass spacer. We notice the increase of the maximum absorption and the wavelength at the maximum compared to the air spacer for $f = 0.5$. However, the maximum absorption may decrease instead for $f = 0.3$. In the case of $a = 7$ nm, the dependence departures from the linear one for the glass spacer covering a wide range of absorption values and keeping the wavelengths at peaks in a narrow band. Such a behaviour might me related to the resonant response of the hypercrystal, when the deviations cease to be incremental.

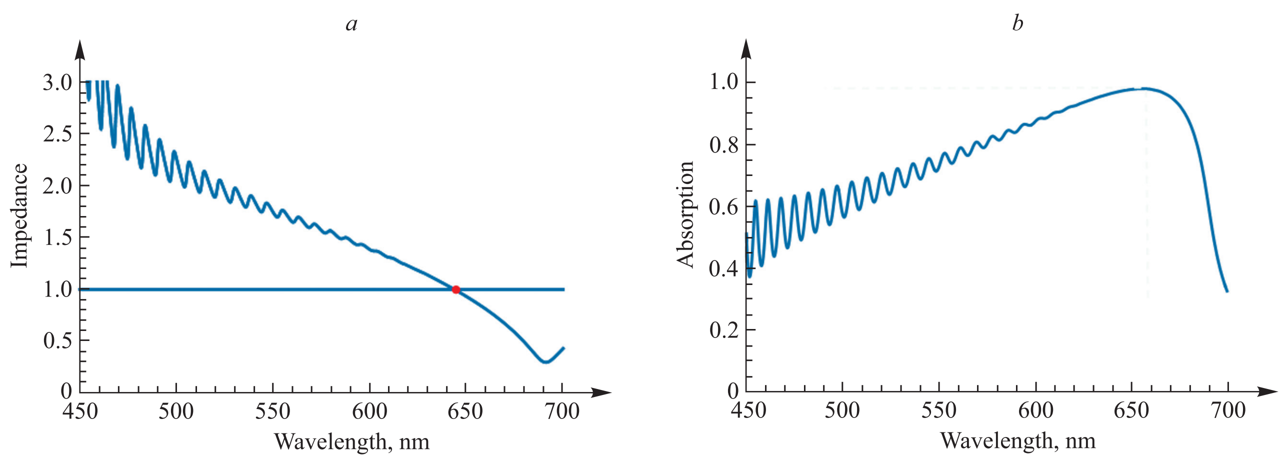

Fig. 3. Real part of the wave impedance (*a*) and absorption spectrum (*b*) of the hypercrystal $((AB)_{10}C)_{40}$, the hypercrystal achieved for the 10 nm thick air spacer and the 9 nm thick HMM unit cell

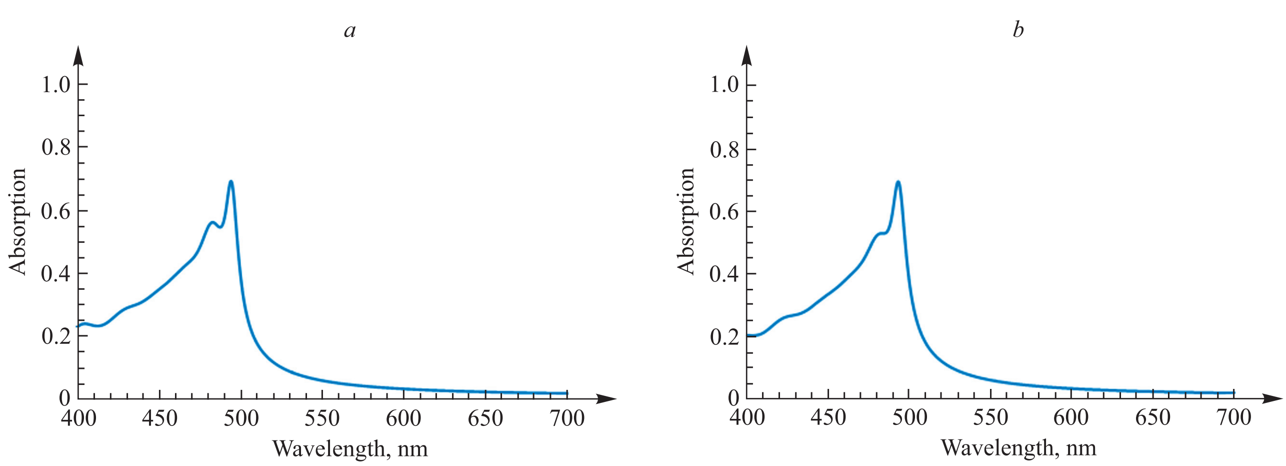

Fig. 4. Absorption spectrum of the HMM composition $(AB)_{70}$ (*a*) and absorption spectrum of the hypercrystal composition $((AB)_{10}C)_7$ (*b*). Dielectric (A) and metal (B) have the same thicknesses 4.5 nm, while the dielectric spacer is 10 nm thick

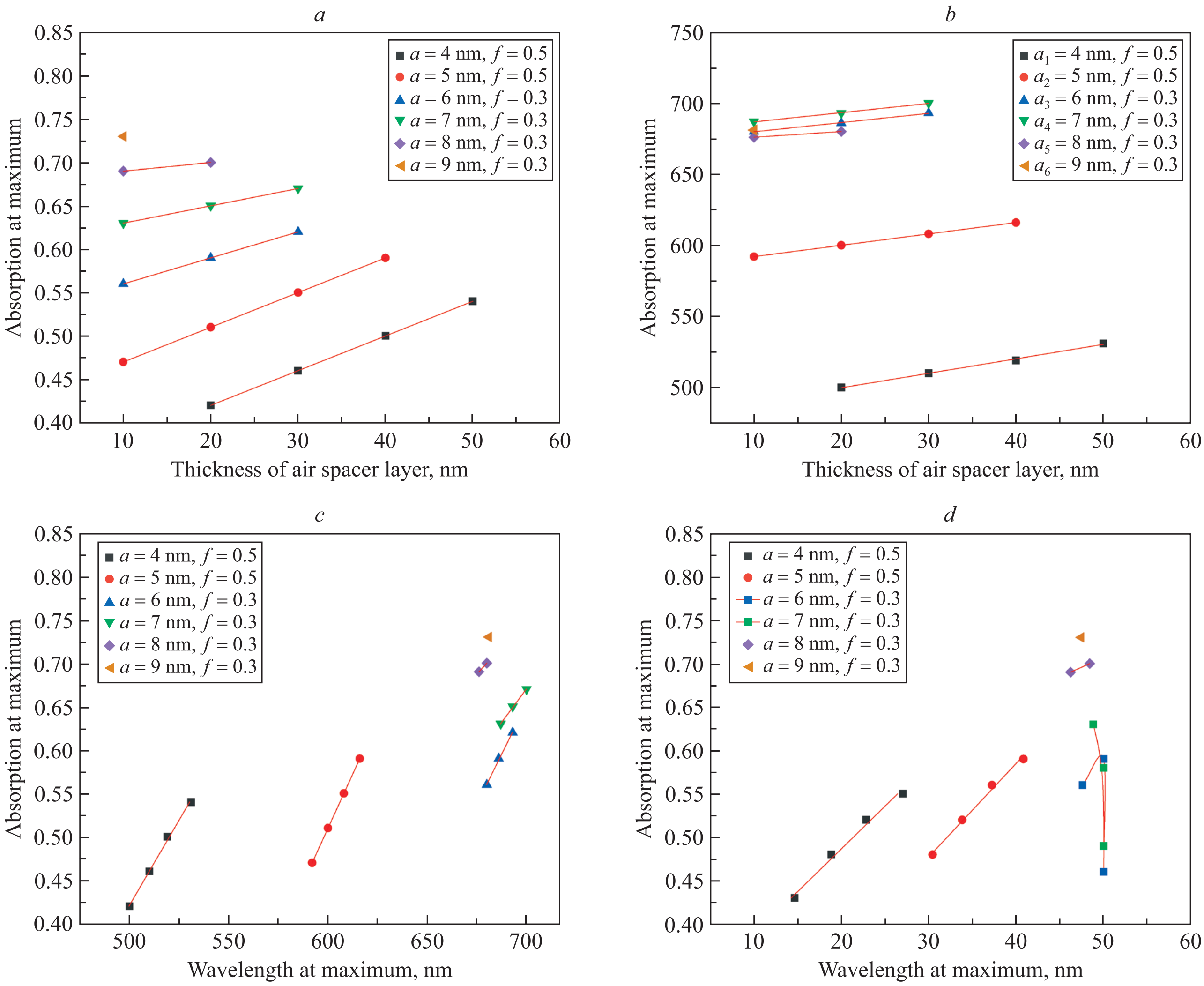

Fig. 5. Absorption (*a*) and wavelength at the maximum (*b*) versus thickness of the air spacer; absorption at maximum versus wavelength at maximum (*c*); comparison of maximum absorption and maximum wavelength between air and glass spacer (*d*)

Absorption spectrum in the case of the maximum absorption for the hypercrystal $((AB)_{10}C)_7$ is depicted in fig. 6, *a*. The half-width at the half maximum of the peak equals 81 nm. The absorption can be enhanced due to the increase of the number of layers in the hyperbolic metamaterial. Indeed, the absorption approaches 0.84 for the structure $((AB)_{20}C)_7$. Such a growth of absorption is associated with the increase of the amount of metal in the system.

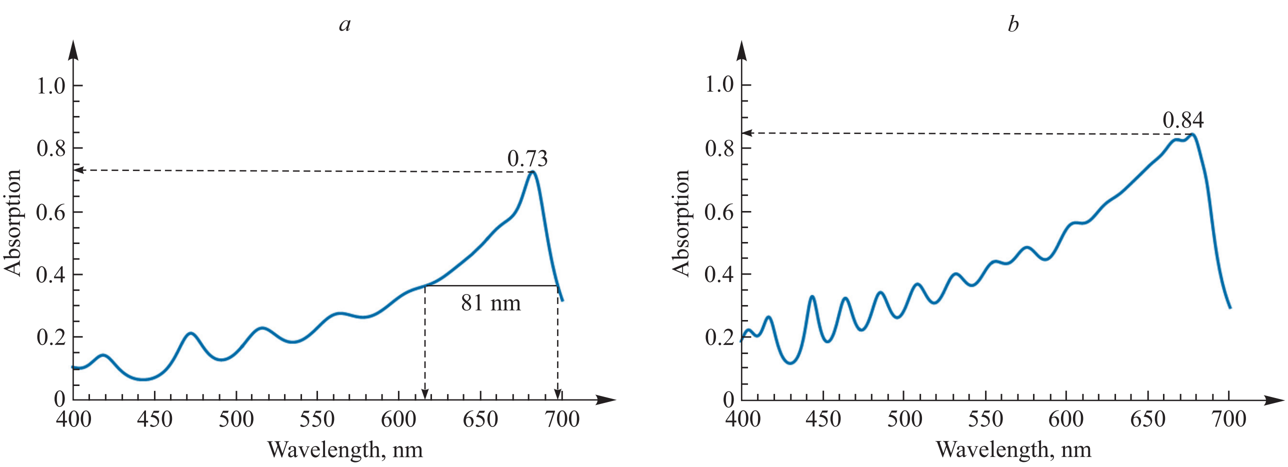

Fig. 6. Absorption spectrum of the hypercrystals $((AB)_{10}C)_7$ (*a*) and $((AB)_{20}C)_7$ (*b*) (dielectric and metal of 6 and 3 nm thickness, air spacer thickness 10 nm)

Conclusions

We have considered hyperbolic metamaterials consisting of alternating silicon and silver layers and periodic hypercrystals comprising these hyperbolic metamaterials and a spacer in the visible spectral range. Using the theory of wave propagation in multilayer systems, we have written the dispersion relation of waves in hypercrystals and demonstrated the appearance of ordinary and extraordinary waves in such an effective anisotropic material. We have revealed the link between the impedance matching condition that suppresses the reflection and absorption peak for a hypercrystal. We have investigated the absorption ability of different compositions of hypercrystals differing with the thicknesses of the silicon, silver and spacer layers. This research might be useful for maximising absorption to achieve a broadband perfect absorber on the hypercrystal platform.

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Received 15.01.2024 / revised 30.01.2024 / accepted 30.01.2024.