ФИЗИКА

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ПАРАМЕТРИЧЕСКОЕ МОДЕЛИРОВАНИЕ ФОТОННЫХ КРИСТАЛЛОВ В ПЕРЬЯХ ПТИЦ

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PARAMETRIC MODELING OF PHOTONIC CRYSTALS IN FEATHERS OF BIRDS

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Исследуются фотонные кристаллы, которые естественным образом встречаются в перьях некоторых видов птиц со структурным типом окраски с точки зрения возможных оптических приложений. Разработана параметрическая трехмерная модель фотонного кристалла, состоящего из твердых цилиндрических меланосом, встроенных в кератиновую матрицу, для изучения того, как геометрия структуры связана с оптическими свойствами. Потенциально ключевые особенности, заложенные природой в дизайн фотонных кристаллов в птичьих перьях, могут быть успешно реализованы технически для датчиков в оптическом диапазоне волн. Возможные сенсорные устройства такого типа могут иметь преимущества из-за низкого энергопотребления, высокой чувствительности, небольших размеров и т. д.

Ключевые слова*: фотонный кристалл, структурная окраска, оптические датчики, отражение.*

The photonic crystals that occur naturally in feathers of some species of birds involving structural type of coloration from the perspective of optical applications are investigated. A parametric 3D model of the photonic crystal composed of solid cylindrical melanosomes embedded in keratin matrix for studying how the geometry of the structure relates to optical properties was developed. Potentially the key features embedded by nature into the design of the photonic crystals in bird's feathers can be successfully technically utilized for sensing application in optical wave range. The possible sensing appliances of this type might advance regarding to low power consumption, high sensitivity, small dimensions etc.

Keywords: *photonic crystal, structural coloration, optical sensors, reflectance.*

Introduction

The realm of birds is extremely diverse – more than 10 000 species of birds are found on our planet. Different species have inherent unique appearance, however from the physical point of view all these colors in birds are created by just two main mechanisms. The first one is pigmental (pigmentary) type of coloration, which is quite simple and well known [1]. Pigments are colored chemical substances that can be found in both plants and animals. The coloration realized by pigments is independent of the structure of the feather. When the outer white light, which is a combination of wavelength from 400 to 750 nm, illuminates the structure of a feather, part of the initial wavelengths is absorbed but part is reflected. We see the reflected light, thus if, for example, only the red wavelength is reflected we see the bird as red.

The second type of coloration – structural coloration – is not so common as pigmental and is divided into two subdivisions: iridescent and non-iridescent [2]. Structurally colored feathers produce their colors by a non-pigmentary way as they are typically made of only few proteins, most commonly, melanin and keratin. The structural color is a result of interference of light on sub micrometer structures inside of the feather. Despite this very limited range of materials involved in structural coloration of birds, the photonic crystals in the structures of feathers produce full range of colors of visible spectrum. Iridescent feathers contain cylindrical rodlets in their structures called melanosomes. For iridescent type coloration, the observable colors are changing at different viewing angles. Tiny spherical air pockets in the feathers can scatter incoming light, resulting in a specific, non-iridescent color. For non-iridescent coloration the color is not changing at different viewing angles and from this point of view it is similar to pigmentary type of coloration. Blue colors in feathers are almost always produced in this manner.

Structural coloration results from the interaction of light waves with featured structures having the same order of size as the wavelength of light. The structures most commonly have a cylindrical or spherical shape. Structural coloration is typically

described by light scattering from a multilayer structure and thin-film interference [3].

1 Setup of the model

To get an insight into the physical mechanism of coloration of birds, we developed a numerical 3D model (using finite element method solver for electromagnetic structures Ansys HFSS 14, which is 3D electromagnetic simulation software for designing and simulating high-frequency electronic products) with material parameters assigned taking into account their dispersive character for every protein involved into the structure. As the model incorporates a number of geometrical parameters influencing the resultant spectral characteristics, we implemented the model to be fully parameterized to make a well-rounded study. In the model of the photonic crystal shown in Figure 1.1, we implement the following main features. The incident light is represented as a plane wave, linearly polarized with two orthogonal polarizations TE and TM. The sources of excitation of these waves in Ansys HFSS are determined by 'Floquet ports' which are located at the top and bottom of the structure in Figure 1.1. There are two pairs of periodic planes along YZ and YX translating the structure along X and Y axes which are set as 'Master' and 'Slave' boundary conditions.

In Figure 1.1, a cross section of a photonic crystal representing the microstructure inside a feather of some birds is shown. Notably, there are only two main material components (keratin and melanin) involved in the structure, which as a whole surrounded by air. In the model, we take into account the dispersion of material parameters for both melanin and keratin and losses of electromagnetic radiation inside the structure. The real part of the wavelength-dependent refractive indices of keratin and melanin, n_k and n_m, was calculated with the Cauchy formula $n = A + B\lambda^{-2}$ (λ is the wavelength of light), using for keratin $A_k = 1.532$ and $B_k = 5890$ nm^2 and for melanin $A_m = 1.648$ and $B_m = 23700$ nm^2; the imaginary component of the refractive index for keratin was assumed to be negligible in the visible wavelength range, but that of melanin was taken to be $k_m = a_m \exp(-\lambda / b_m)$, where $a_m = 0.56$ and $b_m = 270$ nm [4], [5].

The structure of the photonic crystal in Figure 1.1 is limited by the keratin layer (depicted in red), the thickness of which is 3 um. The bottom of the matrix is ragged having a saw-tooth structure which serves as an impedance matching intermediate surface between keratin and air and helps avoiding Fabry – Perot oscillations in reflectance spectra. Initially all the geometrical parameters of the structure in the model are set as default by assigning them as follows: the keratin thickness is 3 um, the thickness of the upper keratin layer is 100 nm, the diameter of melanosomes $D = 100$ nm (they are magnified in Figure 1.1 for convenience), the number of layers is 7, the inter-layer spacing (distance between adjacent layers) $I = 150$ nm, the arrangement of melanosomes represents a rectangular lattice. By default, the model incorporates a normal incidence of light. For the case of an oblique incidence, the TE polarization of electric field is in the YZ plane and TM polarization is along the X-axis.

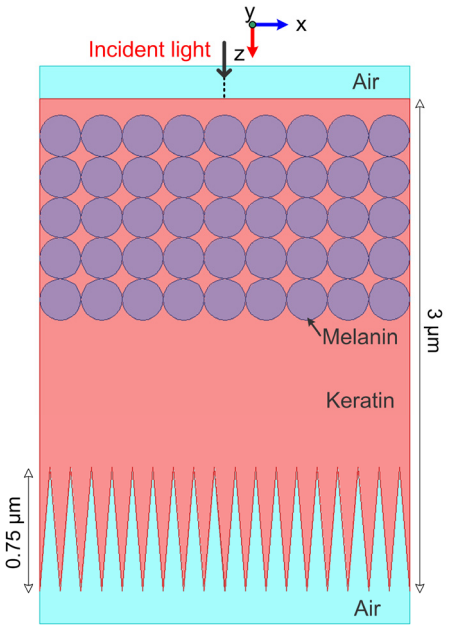

Figure 1.1. – Schematic of an array composed of solid melanosomes immersed in keratin matrix nside a feather's barbule of some birds with specific structural type of coloration

The structure we study in Figure 1.1 is actually represents half of the real structure found in barbules of feathers. However the reflectance from the half of the structure very closely follows the reflectance from the full structure of the double-stacked photonic crystal. In the real structure of a photonic crystal in bird feathers, the rows of melanosomes are not ideally arranged, and the diameters of the melanosomes differ slightly from each other. The imperfections lead to reducing the peak reflectance leaving the shape of the spectra virtually the same [6].

2 Results of modeling

We start our analysis of reflectance spectra by varying value of the number of melanosome layers. Figure 2.1 (a, b) shows that with increasing the number of layers an obvious increase in peak reflectance is observed, the bandwidth slightly narrows and a small bathochromic (towards longer wavelengths) peak shift occurs. Despite we applied the impedance-matching surface for the bottom keratin surface, the tiny high-frequency oscillations in spectra in Figure 2.1 (a, b) are still visible for the cases of pure keratin matrix and for unitary and triple layer(s) of melanosomes, however the oscillations completely disappear for higher number of melanosomes in the stack, as it is shown for 5 layers.

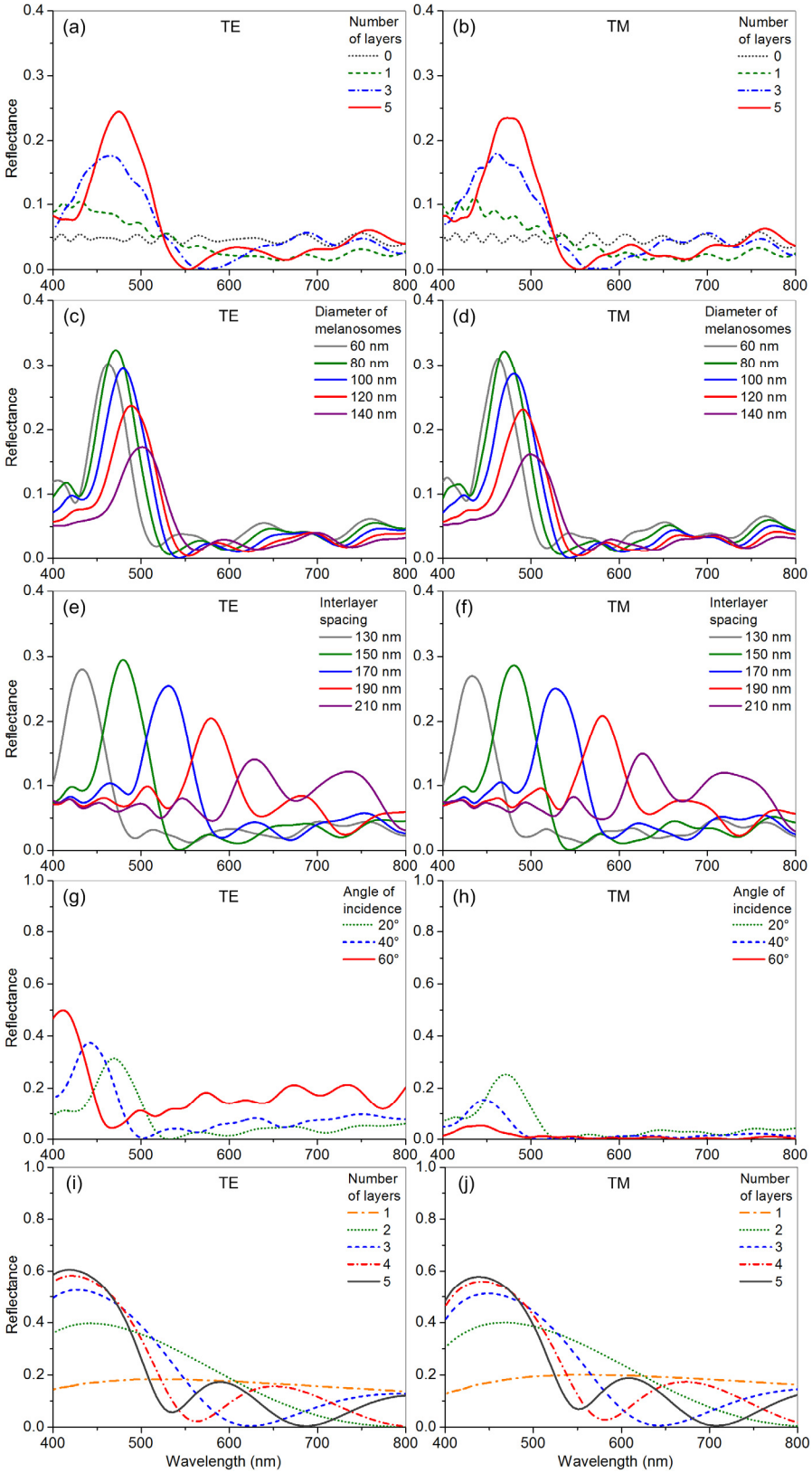

Figure 2.1. – Results of modeling. (a, b) Reflectance spectra vs. number of layers in the array; (c, d) Reflectance spectra vs. diameter of melanosomes; (e, f) Reflectance spectra vs. inter-layer spacing (distance between centers of adjacent layers); (g, h) Reflectance spectra vs. angle of incidence. The case of normal incidence (0°) was considered in figures (e–f); (i, j) Reflectance spectra vs. number of layers for the case when the keratin layer is replaced by the air. In the case of (c, d, e, f, h) the number of layers of melanosomes was seven

The diameter of melanosomes is one of the key parameters which strongly influences the perk reflectance while causing only slight changes in the peak wavelength positioning. Figure 2.1 (c, d) demonstrates the reflectance dependence on the diameter of melanosomes and indicates that the dependence is not monotonous: with increasing the diameter of cylinders the reflectance first increases reaching its peak at 80 nm and then changes the trend into opposite decreasing almost twice at 140 nm from its peak value.

The dependence of reflectance on interlayer spacing (which is a distance between adjacent layers of melanosomes) is radically different from the dependence on diameter of melanosomes from the point of view of the peak shift. As Figure 2.1 (e, f) shows, in this case both the peak wavelenth positioning and peak shift are strongly depending on the parameter of interlayer spacing. The peak of reflectance reaches its maximum at 150 nm at which the stack of melanosomes is closely packed as the interlayer spacing is also (as default) has the length of 150 nm. This behavior can be interpreted with the following rule $\lambda_{\max} = 2\left(n_1 d_1 + n_2 d_2\right)$ for a multilayer composed of two components with refractive indices n_1 and n_2 and thicknesses d_1 and d_2. As an example, taking $n_1 = 1.55$ and $n_2 = 1.65$ and $d_1 = d_2 = 75$ nm (half of the interlayer spacing at close packing), yields $\lambda_{\max} = 480$ nm. Higher (lower) values of the wavelengths will result to an increasing (decreasing) multilayer period. We must emphasize, however, that light interference in the combined structure consisting of the upper thin-film-like keratin cortex and the multilayer stack of melanosomes ultimately determines the reflectance spectrum. Increasing the interlayer spacing leads to reduction in the peak magnitude, which almost decreases twice at 210 nm and to changing in the shape of the spectrum, which transforms substantially into two-peak profile.

To study the iridescent properties of the photonic crystal, we performed angle dependence analysis for TE and TM modes. Figure 2.1 (g, h) reveals the peculiarities of spectra transformations with increasing the incidence angle. First of all, the TE and TM spectra differ strongly from the point of view of the peak height but have the same trend for the peak shifting. From the peak shift, it definitely follows that the appearance of the structure will acquire a purplish tint with observing at oblique angles.

The total reflectance of the spectra we have just analyzed is not impressively high staying in its peak on the level of 30% which might not be sufficient at some image or sensing applications but seems to be quite enough for color signalling in birds' communications. The reason for that lays in low refractive index contrast between melanin and keratin. To demonstrate the potential ability of increasing the peak reflectance in some artificial photonic crystals based on the same principle, we replaced the keratin matrix by air for studying the increment of reflectance. Figure 2.1 (i, j) depicts the reflectance spectra in this case when the melanosomes are surrounded by air. First, one can see that the spectra became wider and, second, the peak reflectance doubled in comparison with reflectance in Figure 2.1 (a, b).

It is necessary to note, that there is one more parameter that influences both peak reflectance and peak wavelength. The parameter is the thickness of the upper-keratin layer or keratin cortex, which is the distance between the top keratin surface the upper layer of melanosomes. With increasing cortex thickness both the peak reflectance and peak wavelength also increases.

Conclusion

Full parametric analysis of a photonic crystal found in birds feathers reveals details of the physical mechanism of colors formation in this type of photonic crystals. The type of photonic crystal utilizes materials with very limited refractive index contrast, therefore, it is reasonable to continue our modeling by considering more complicated photonic crystal with hollow melanosomes [7]. The knowledge obtained in this analysis can be applied at the stage of designing photonic optical sensors, indicators, displays with new types of light reflectors with reconfigurable spectrum and almost zero power consumption, metamaterials [8]–[12]. As our analysis indicates, the number of layers of cylinders in the photonic crystal for satisfactory spectra recognition (or formation) can be limited by just 5–7 layers. The best parameter for the reflecting color controlling in the photonic crystal is the interlayer spacing while the diameter of cylindrical melanosomes is responsible for the magnitude of the peak reflectance.

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