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PHYSICS

Effect of Long-Period Ordering of the Structure of a Plant on the Initial Stages of Photosynthesis

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Abstract—Using data on the structure of plant leaves, specific features of light propagation in biophotonic-crystal structures have been established by the transfer matrix method. Splitting of the stopband in two bands has been found. The density of photonic states and the electromagnetic field value have been calculated. The occurrence of two photosystems (splitting of the stopband in two bands), the peculiarity of the long-wavelength quantum yield and its enhancement (Emerson effect), and water dissociation in the soft mode due to an increase in the electromagnetic field on the layers are explained.

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Since the discovery of photosynthesis, this phenomenon has intrigued researchers [1–3] due to the unique ability of plants, seaweed, and cyanobacteria to convert the energy of light into chemical compounds. The development of experimental techniques drastically changed the concepts on the mechanisms of this process [4]. The process of photosynthesis is conventionally divided into three stages.

The first stage is absorption of light. The second stage is conversion of the energy of light into electrostatic energy of separated proton and electron charges forming upon water splitting. This energy transforms to the energy of chemical bonds of the organic substances forming in plants, including adenosinetriphosphoric acid molecules. The third stage is conversion of CO_2 into carbohydrates.

According to the current concepts [4, 5], the process of photosynthesis occurs in photosystems 1 and 2.

The pigment complex consisting of chlorophyll molecules (a and b), proteins, carotinoids, and phycobilins works as a system absorbing the energy of light quanta and transferring it to the reaction center. In this case, the production of one oxygen molecule requires, according to various data [4], from 300 to 5000 chlorophyll molecules. The structure of these complexes and mechanisms of the excitation energy transfer are still under dsicussion.

It is interesting to consider a specific feature of the wavelength dependence of the quantum yield (the ratio between absorbed light quanta to the amount of oxygen released). At wavelengths over 685 nm, it sharply decreases, although chlorophyll still absorbs in this range. This phenomenon is called the red drop. Under illumination by two waves at 700 and 650 nm, the efficiency of photosynthesis grows (the Emerson effect) [2]. The nature of this phenomenon has not been determined theoretically. The correlation between the plant structure and optical properties has not been established either.

It was found that plant leaves consist of structural elements characterized by long-period ordering and representing layers with different permittivities [6, 7].

In the literature, such structures are called photonic-crystal structures or, as applied to biological objects, biophotonic-crystal structures. In the latter case, the ordering is hidden [7]. The spectrum of electromagnetic waves in such structures consists of bands. The presence of photonic bands (stopbands) allows the rate of optical radiation of atoms and molecules to be controlled [8]. At the stopband edges, the electromagnetic field multiply increases [9]. The photonic-crystal structure can contain defects that break its periodicity and lead to the occurrence of defect frequencies (so-called defect modes) lying in the band gaps. The density of photonic states for these modes is significantly higher [9, 10].

Certainly, the drastic changes in the spectral characteristics of light waves propagating in plant leaves affect the initial stages of photosynthesis.

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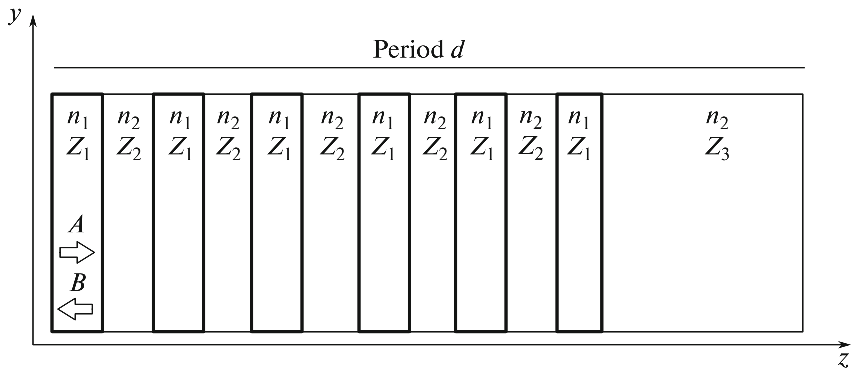

Fig. 1. Long-period structure with period d and sublattices with refractive indices n_1 and n_2, which simulates the structures of natural objects.

In view of the aforesaid, this study was aimed at establishing the effect of a long-period structure with a defect on the optical properties and local characteristics of light waves propagating in a sample.

In this work, we used the transfer matrix method [10] for calculating the transmission and reflection spectra on the basis of structural data and establishing the electromagnetic field distribution in a layered structure.

One of the best-studied among these structures is a begonia plant [7] and cyanobacteria with a similar structure.

Figure 1 shows a model of the layered structure of plant cells (chloroplasts). The begonia iridoplasts have an analogous structure [7].

In a medium consisting of layers with thickness Z_N and refractive index n_N, a plane electromagnetic wave propagates. Its incidence plane is yz. The structure has period d and contains two sublattices with refractive indices n_1 and n_2 (Fig. 1). The amplitudes of waves A and B, which propagate in the previous layer in the right- and left-hand direction, respectively, depend on the same values in the current layer [10]:

$$A_{N-1} = \frac{1}{2}((1+C)A_N e^{-ik_N z_N} + (1-C)B_N e^{ik_N z_N}),$$
$$B_{N-1} = \frac{1}{2}((1-C)A_N e^{-ik_N z_N} + (1+C)B_N e^{ik_N z_N}). \quad (1)$$

For the TE mode (the electric component is perpendicular to the incidence plane), we have

$$E(z,N) = (A_N^{\mathrm{TE}} e^{-ik_N z} + B_N^{\mathrm{TE}} e^{ik_N z}),$$
$$H(z,N) = ik_N (A_N^{\mathrm{TE}} e^{-ik_N z} - B_N^{\mathrm{TE}} e^{ik_N z}), \quad (2)$$
$$C = \frac{k_N}{k_{N-1}}.$$

For the TM mode,

$$H(z,N) = (A_N^{\mathrm{TM}} e^{-ik_N z} + B_N^{\mathrm{TM}} e^{ik_N z}),$$
$$E(z,N) = i\frac{n_N^2}{k_N}(A_N^{\mathrm{TM}} e^{-ik_N z} - B_N^{\mathrm{TM}} e^{ik_N z}), \quad (3)$$
$$C = \frac{k_{N-1} n_N^2}{k_N n_{N-1}^2};$$
$$k_N = \frac{\omega}{c}\sqrt{n_N^2 - n_0^2 \sin^2\theta}, \quad (4)$$

where Z is the local variable for each layer with the reference point placed on the right-hand layer boundary and θ is the angle of incidence of the beam from the environment.

Under normal incidence of light, i.e., $k_N = \omega n_N/c$, Eqs. (2) and (3) become identical.

Knowing that there is only an outgoing wave (A_{out}; $B_{\mathrm{out}} = 0$) at the structure output, we can compute an array of relative amplitudes in each photonic-crystal layer.

The transmittance is

$$T = 1 - \left|\frac{B_0}{A_0}\right|^2. \quad (5)$$

In addition, these computations allowed us to determine the electromagnetic field distribution in the layered structure.

Figure 2 (*1*) shows the calculated spectrum of a defect-free structure from Fig. 1 with the parameters taken from study [11]. It is worth noting that the refractive indices of natural objects have low contrast [12]. Nevertheless, the spectrum of electromagnetic waves has a band structure. The density of photonic states $\rho(\lambda)$ for this structure (Fig. 2 (*2*)) is enhanced at the stopband edges.

It can be seen in Fig. 2 (*1*) that the radiation of atoms or molecules in the wavelength range from 460 to 560 nm is complicated, since the molecules excited

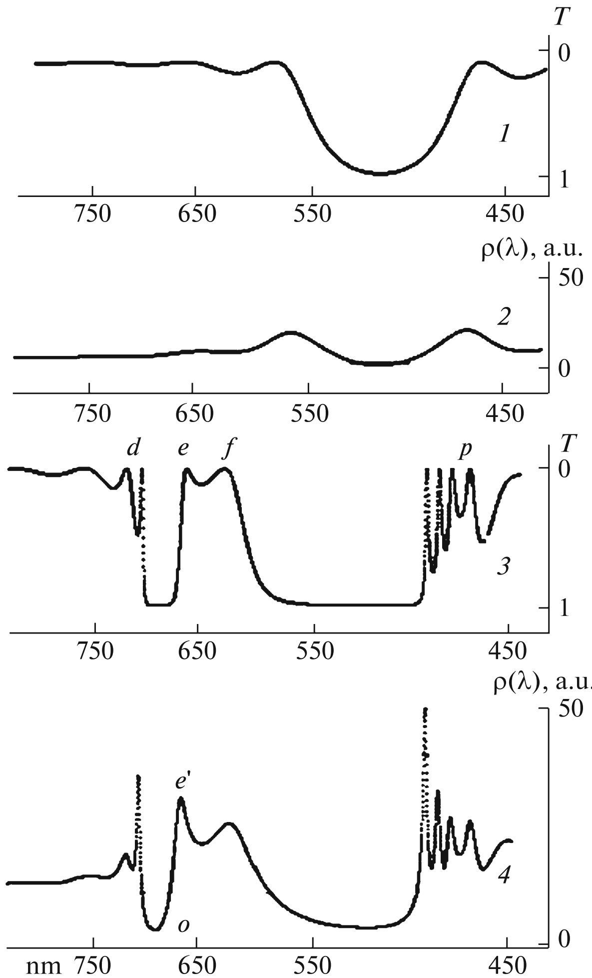

Fig. 2. (*1*) Transmission spectrum of the defect-free structure (Fig. 1), (*2*) density of photonic states (ρ(λ)), and (*3*) transmission spectrum of the structure with regard to the chlorophyll *b* absorption lines and (*4*) the density of photonic states (ρ(λ)).

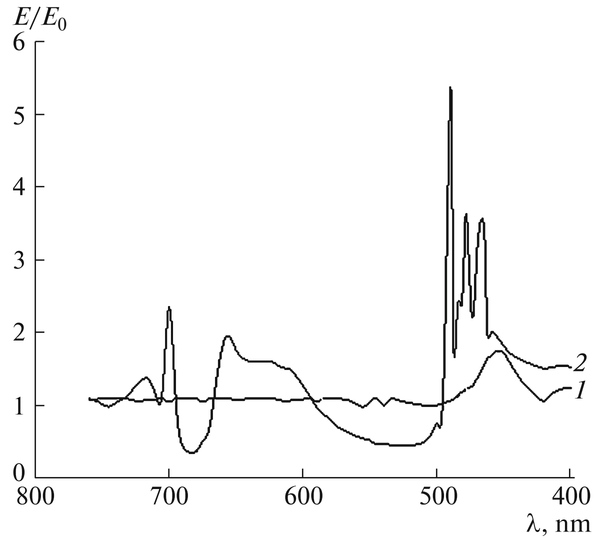

Fig. 3. (*1*) Frequency dependence of the maximum electromagnetic field on the central layer for the ordered structure (Fig. 2 (*1*)) and (*2*) the structure with regard to the chlorophyll absorption lines *b* (Fig. 2 (*3*)).

by light with a wavelength of 460 nm fluoresce according to the Stokes rule at larger wavelengths hitting the stopband. In addition, the stopband includes chlorophyll absorption lines a and b. In this case, there is a strong interaction between the exciton and Bragg resonances [13].

The results of the calculation with regard to the chlorophyll absorption spectrum are presented in Fig. 2 (*3*).

Comparison of Figs. 2 (*1*) and 2 (*3*) shows the changes in the stopband. It is broadened and additional modes occurred, which are caused by structural defects.

In this case, the density of photonic states (Fig. 2 (*4*)) is higher than that of the ordered structure (Fig. 2 (*2*)).

The entire stopband is divided into two parts (*de* and *fp*). The red drop of the quantum yield is caused by a decrease in the density of photonic states in this wavelength range (*e'o*) (Fig. 2 (*4*)). In addition, this figure elucidates the origin of Emerson enhancement. Under irradiation of molecules by light with wavelengths in the range (*ef*), the excited photons from (*fp*) are thrown to the part of range (*de*). Then, the photosynthesis quantum yield in the red spectral range grows.

Figure 3 shows the frequency dependence of the electromagnetic field maximum in the central layer for the ordered structure (*1*) (Fig. 2(*1*)) and the structure with regard to the chlorophyll absorption lines (*2*) (Fig. 2 (*3*)). One can see the increase in the electromagnetic field at the stopband edges.

Thus, the calculated data on the optical properties of long-period plant structures makes it possible to explain the peculiarities of the initial photosynthesis stages using a unified approach, specifically, (i) the occurrence of stopbands, (ii) the occurrence of two photosystems (separation of the stopband in two bands), (iii) the peculiarity of the long-wavelength quantum yield, i.e., its weakening under irradiation by light in the range from 685 to 710 nm and enhancement under additional irradiation near 650 nm (Emerson effect), and (iv) water dissociation in the soft mode due to the increase in the electromagnetic field on the layers.

In addition, our results explain the shift of the red boundary of water dissociation toward longer wavelengths in the quasi-ordered structures [14] as compared with structures with a small period and the decrease in the voltage required for water dissociation in chloroplasts under their irradiation [15].

Our results are consistent with the chemiosmotic Mitchel theory [2] about the mechanisms of energy conversion in biological membranes. The energy storage in adenosinetriphosphoric acid occurs through preliminary charge accumulation on the membrane walls. The difference between electrochemical potentials of hydrogen ions on conjugating membranes, i.e., inner membranes of mitochondria, thylakoids, and chloroplasts, is caused by the light quanta absorbed.

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