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Absorption characteristics of bacteriorhodopsin molecules

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Abstract. The bacteriorhodopsin molecule absorbs light and undergoes a series of structural transformation following a well-defined photocycle. The complex photocycle is transformed to an equivalent level diagram by considering the lifetime of the intermediate states. Assuming that only B and M states are appreciably populated at any instant of time, the level diagram is further simplified to two-level system. Based on the rate equations for two-level system, an analytic expression for the absorption coefficient of bacteriorhodopsin molecule is derived. It is applied to study the behaviour of absorption coefficient of bacteriorhodopsin film in the visible wavelength region of 514 nm. The dependence of absorption coefficient of bacteriorhodopsin film on the thickness of the film, total number density of active molecules and initial number density of molecules in B-state is presented in the graphical form.

Keywords. Slow saturable absorber; photocycle; two-level system; biomolecule.

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Among the biological materials proposed for photonic applications [1–6], bacteriorhodopsin (BR), a pigment in purple membrane of salt-loving bacteria called halobacteria is an outstanding candidate [7]. The BR molecules absorb light and undergo a series of structural transformation following a well-defined photocycle [8] and it can be described by an equivalent level diagram (figure 1) in which the intermediate J-state is neglected because of its femtosecond lifetime.

In this article the analytical expression for the absorption coefficient of BR molecules [9] is used to obtain the double pass absorption coefficient of BR films and it is applied to study the dependence on the system parameters. The results and discussions are presented in the graphical form. This study finds importance in generation of ultrashort pulses of femtosecond duration by passive mode locking of lasers, wherein the pulse duration depends on the selective saturable absorption coefficient of the saturable absorber, which is free from photodegradation.

The levels B and M are assumed to be appreciably populated at any instant of time. This has made the equivalent level diagram to reduce to simple two-level system as shown in figure 2. The population density of B and M states are assumed to be $B(t)$ and $M(t)$ at any instant of time. By solving the rate equations for the two-level system of BR, the absorption coefficient of BR molecules is of the form [9]

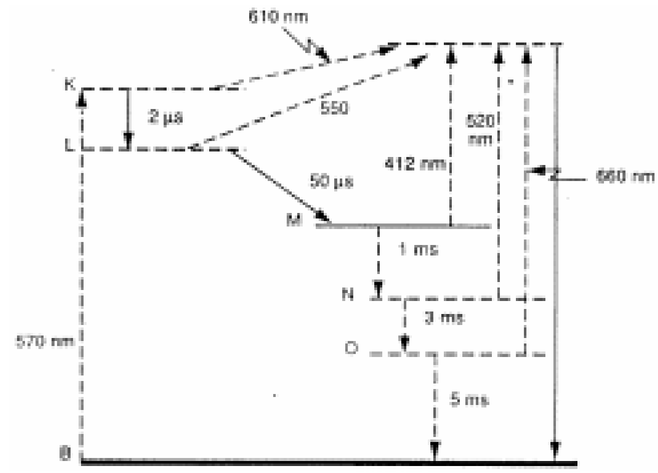

Figure 1. Equivalent energy level diagram of photocycle of BR molecule.

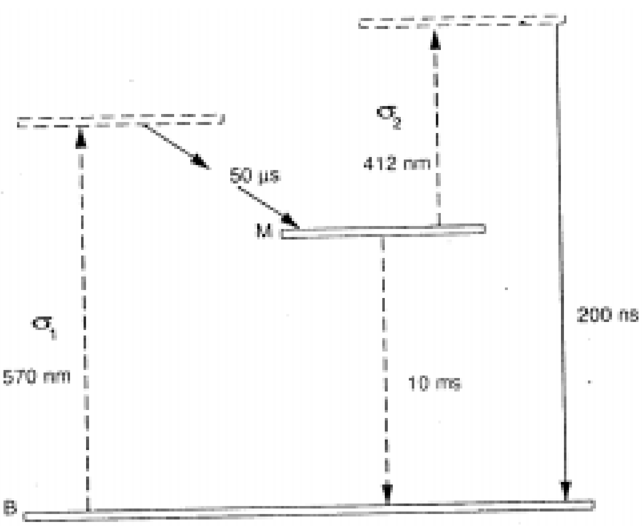

Figure 2. Simplified energy level diagram of photocycle of BR molecule.

$$\alpha(t) = \frac{2\sigma_1\sigma_2 N}{\sigma_1+\sigma_2} + \frac{(\sigma_2-\sigma_1)\sigma_2 N}{\sigma_1+\sigma_2} - \left[\left\{\frac{(\sigma_2-\sigma_1)\sigma_2 N}{\sigma_1+\sigma_2}\right\} - (\sigma_2-\sigma_1)B_{\mathrm{i}}\right]\bar{E}$$
$$+\frac{1}{2}\left[\left\{\frac{(\sigma_2-\sigma_1)\sigma_2 N}{\sigma_1+\sigma_2}\right\} - (\sigma_2-\sigma_1)B_{\mathrm{i}}\right]\bar{E}^2 - (\sigma_2-\sigma_1)B_{\mathrm{i}}, \qquad (1)$$

where $\bar{E} = E(t)/E_s$, σ_1 and σ_2 are the absorption coefficients of levels B and M respectively, $N = B(t) + M(t)$ is the total number density of BR molecules, B is the initial number density of the active BR molecules before the arrival of the pulse in the level B. $E(t) = \int_0^t |v(t')|^2 \, \mathrm{d}t'$ is the cumulative energy in the pulse where $v(t')$ is the amplitude of the electric field. $E_s = [h\nu A_s/(\sigma_1 + \sigma_2)]$ is the saturation energy parameter of the slow saturable absorber.

Since the mode-locked pulse in the laser cavity makes to and fro journey, it gets modified twice in a round-trip. Hence the double pass absorption coefficient of BR film is considered and it is given by

$$S(t) = \alpha(t) 2l_s, \tag{2}$$

where l_s is the thickness of BR film.

The analytical expression for the absorption coefficient of BR film is applied to study the absorption characteristics of BR molecules in a typical laser system operating at fundamental wavelength 514 nm. The experimental data available for the absorption coefficients of the levels B and M corresponding to the wavelength 514 nm are $\sigma_1 = 1.55 \times 10^{-16}$ cm^2 and $\sigma_2 = 1 \times 10^{-18}$ cm^2 respectively [10] are employed in the parametric analysis and the thickness of the BR film is taken as 100 μm [9]. Since the experimental results are not reported elsewhere, comparison between the experimental and theoretical results has not been made. Further, the details of laser powers used and energy measurement techniques are not involved in this analytical work.

The dependence of $S(t)$ on l_s for $B_{\mathrm{i}} = 0.5 \times 10^{16}$ molecules/cc and different values of $N = (2.0, 2.5, 3.0, 3.5$ and $4.0) \times 10^{16}$ molecules/cc is shown in figure 3. It shows that $S(t)$ increases rapidly for smaller value of thickness of BR film ranging from 10 to 100 μm and later its dependence with l_s becomes less significant. Also, $S(t)$ is almost invariant with N. This study has provided a valuable information that $S(t)$ varies linearly up to a thickness of 50 μm and later its variation becomes non-linear.

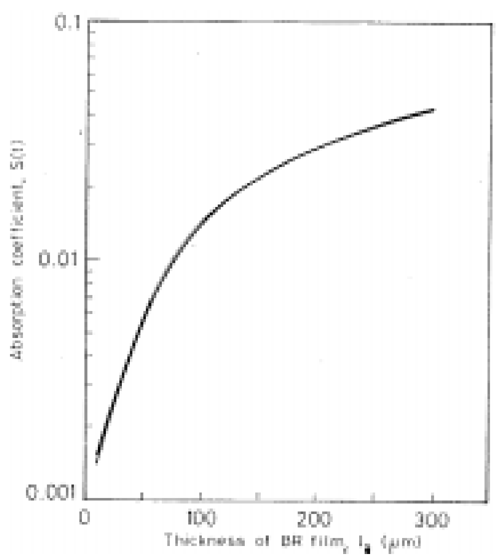

Figure 3. Dependence of absorption coefficient, $S(t)$, on thickness of BR film, l_s, for $B_{\mathrm{i}} = 0.5 \times 10^{16}$ molecules/cc, and different values of N varying from 2.0×10^{16} to 4.0×10^{16} molecules/cc in steps of 0.5×10^{16} molecules/cc.

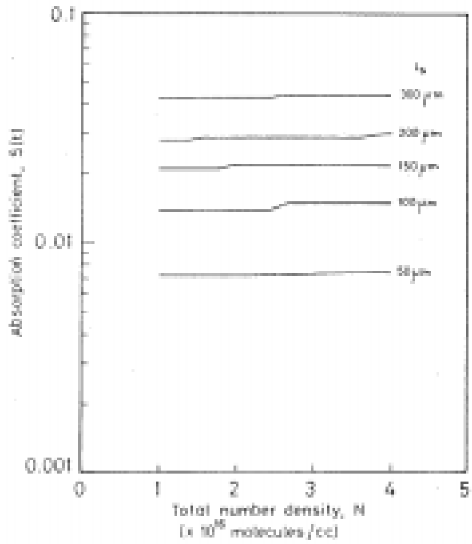

Figure 4. Dependence of absorption coefficient, $S(t)$, on total number density, N, for $B_{\mathrm{i}} = 0.5 \times 10^{16}$ molecules/cc, and different values of l_s.

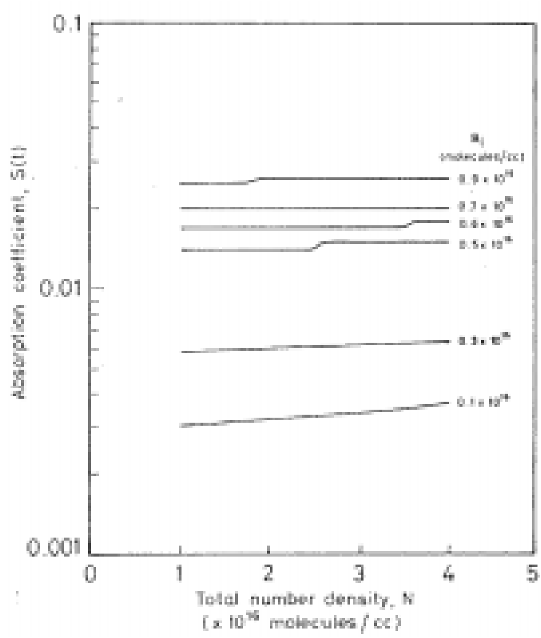

Figure 5. Dependence of absorption coefficient, $S(t)$, on total number density, N, for $l_s = 100$ μm, and different values of B_{i}.

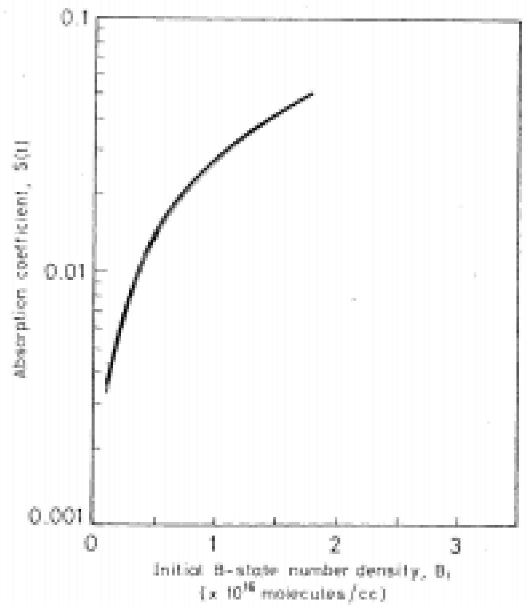

Figure 6. Dependence of absorption coefficient, $S(t)$, on initial B-state number density, B_{i}, for $l_s = 100$ μm, and different values of N varying from 2.0×10^{16} to 4.0×10^{16} molecules/cc in steps of 0.5×10^{16} molecules/cc.

The dependence of $S(t)$ on N, for $B_{\mathrm{i}} = 0.5 \times 10^{16}$ molecules/cc and different values of $l_s =$ 50, 100, 150, 200 and 300μm is shown in figure 4. It is clear that $S(t)$ value is constant for $l_s = 50\,\mu$m. But for other values of $l_s, S(t)$ is constant with a step at certain value of N. This result has predicted that $S(t)$ is independent of N for different l_s keeping B_{i} constant.

The dependence of $S(t)$ on N, for $l_s = 100$ μm and different values of B_{i} =(0.1, 0.3, 0.5, 0.6 and 0.9) $\times 10^{16}$ molecule/cc is depicted in figure 5. It is observed that $S(t)$ increases with increase of B_{i} for its smaller values and it remains almost constant for values greater than 0.5×10^{16} molecules/cc, showing that the variation of $S(t)$ with N is insignificant. This information has provided a novel information to the experimental researcher to select the B-state number density of active BR molecules to achieve the constant value of absorption coefficient of BR film for known thickness.

Finally, the dependence of $S(t)$ on B_{i}, for $l_s = 100$ μm and for different $N =$ (2.0, 2.5, 3.0 and 3.5) $\times 10^{16}$ molecules/cc is presented in figure 6. It is seen that the variation of $S(t)$ is insignificant with N.

To conclude, the absorption characteristics of BR molecules are analysed using a two-level approximation to the complex photocycle. In this analysis it is assumed that only the initial B and intermediate M states are appreciably populated. A simple analytical expression for the absorption coefficient of BR molecules is derived. The dependency of the absorption coefficient on thickness of the BR film, the total number density of active BR molecules and the initial number density of B-state are analysed. The dependence of absorption characteristics on the host matrix is not considered in the analysis because of its thickness of few micrometers.

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