# SIMULATION OF ANGULAR REGULARITIES OBSERVED IN THE SPECTRA OF LIGHT REFLECTED BY THREE-LAYER PLANE STRUCTURES WITH A FABRY-PEROT RESONATOR

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The theoretical simulation of angular regularities observed in the spectra of light reflected by three-layer plane structures with a Fabry—Perot resonator has been carried out. It has been shown that, for the frequencies of light waves beyond the range of longitudinal-transverse splitting, the method of envelope functions, the latter being the values of energy reflection coefficients and phases at the extrema of the interference bands, describes these regularities correctly. It has been established that, for the light frequencies within the range of longitudinal-transverse splitting, one can observe the polarization inversion of the Brewster effect, which depends on the relation between the parameters of media that make up the structure.

## 1. Introduction and Formulation of the Problem

In spite of the fact that the geometry of oblique reflection and transmission of light by three-layer structures with a Fabry—Perot resonator was investigated in many works and became a basis for the known method of ellipsometry [1], the researches carried out recently in optics [2–6] and acoustics [7] evidence for both the existence of a number of unresolved problems and the perspectives for the development of new approaches. For example, in works [8, 9], the thicknesses of superthin layers were suggested to be determined from the measurements of the angle of observation of the Brewster effect (the reflection coefficient $R = 0$) or quasi-effect ($R \to \min$). These phenomena manifest themselves mainly in the $p$-component of polarization [10]. Although, at certain relations between structure parameters, the minimum or the zero value of the reflection coefficient can be obtained in the $s$-polarization as well (see [3 in work [10]]).

From this point of view, it was of great interest to study the opportunity to describe the angular regularities of amplitude-phase spectra using the method of envelope functions, which became the purpose of this work. The envelope functions are the values of the energy reflection coefficient and the phase at the extrema of interference bands. The method of envelope functions has been substantiated by us earlier [11, 12] for normal reflection. In this work, we will show that, in the geometry of oblique reflection, the method of envelope functions correctly describes the amplitude and phase spectra for light frequencies beyond the range of longitudinal-transverse splitting $\omega_0 < \omega < \omega_L$. In the frequency interval $\omega_0 < \omega < \omega_L$ of longitudinal-transverse splitting of the resonant state, a polarization inversion of the Brewster quasi-effect for the $p$-component into the Brewster effect for the $s$-one appears at the frequency of phase compensation [13]. It has also been established that, contrary to the statement made in work [10], the exact equality $R = 0$ cannot be obtained for the $p$-polarization in principle, because this component of the light wave undergoes the additional phase shift by $\pi$ when crossing the Brewster value of the angle of incidence.

## 2. Results and Their Discussion

It is known [14] that, irrespective of the polarization state and the angle of incidence $\alpha$ of the light beam on an interface, the amplitude of the Fresnel factor for a three-layer structure is

$$\tilde{r} = \frac{\tilde{r}_{12} + \tilde{r}_{23} \exp\left(-i\,\tilde{\delta}\right)}{1 + \tilde{r}_{12}\,\tilde{r}_{23} \exp\left(-i\,\tilde{\delta}\right)}, \quad (1)$$

where $\tilde{r}_{12}$ and $\tilde{r}_{23}$ are the amplitudes of the Fresnel factors for the vacuum—film and film—substrate interfaces, respectively. The refractive indices of semi-confined media that contact with a resonator are $n_{1,2}$. The algorithm of calculations of the light wave phase was constructed according to the known conclusion [14] that, at an arbitrary angle $\alpha$ for the $s$-polarization and at an angle $\alpha$ larger than the Brewster one for the $p$-component, the reflected wave undergoes the additional phase variation by $\pi$.

In the cases of both oblique and normal reflections, the angular spectrum is described by the relations

$$R = \frac{R_{\min} + b^2 \cos^2 \frac{\phi_{12} - (\phi_{23} - \delta)}{2}}{1 + b^2 \cos^2 \frac{\phi_{12} + (\phi_{23} - \delta)}{2}} =$$

$$= \frac{R_{\max} - a^2 \sin^2 \frac{\phi_{12} - (\phi_{23} - \delta)}{2}}{1 - a^2 \sin^2 \frac{\phi_{12} + (\phi_{23} - \delta)}{2}}, \quad (2)$$

where $a = \frac{2\sqrt{\sigma_{12}\sigma_{23}}}{1+\sigma_{12}\sigma_{23}}$ and $b = \frac{2\sqrt{\sigma_{12}\sigma_{23}}}{1-\sigma_{12}\sigma_{23}}$. Their envelope functions are (Fig. 1)

$$R_{\min} = \left[\frac{\sigma_{12} - \sigma_{23}}{1 - \sigma_{12}\sigma_{23}}\right]^2, \; R_{\max} = \left[\frac{\sigma_{12} + \sigma_{23}}{1 + \sigma_{12}\sigma_{23}}\right]^2, \quad (3)$$

i.e. the values of the reflection coefficients at the extrema of the Fabry—Perot interference bands, because no restriction was imposed when those expressions were derived in the case of normal incidence of a beam on the interface [12, 13]. The correctness of such an approach for the description of angular regularities of amplitude-phase spectra is illustrated in Fig. 1.

In the case of transparent structure, as follows from formulae (1) and (2), possible are those angles of incidence $\alpha_{12}$ and $\alpha_{23}$, for which the conditions $\mathrm{Re}\,\tilde{r}_{12,23} = 0$ are satisfied. For symmetric structures, $n_1 = n_2$, so that $\alpha_{12} = \alpha_{23}$. But these values of angles cannot be used for a determination of the layer thickness,

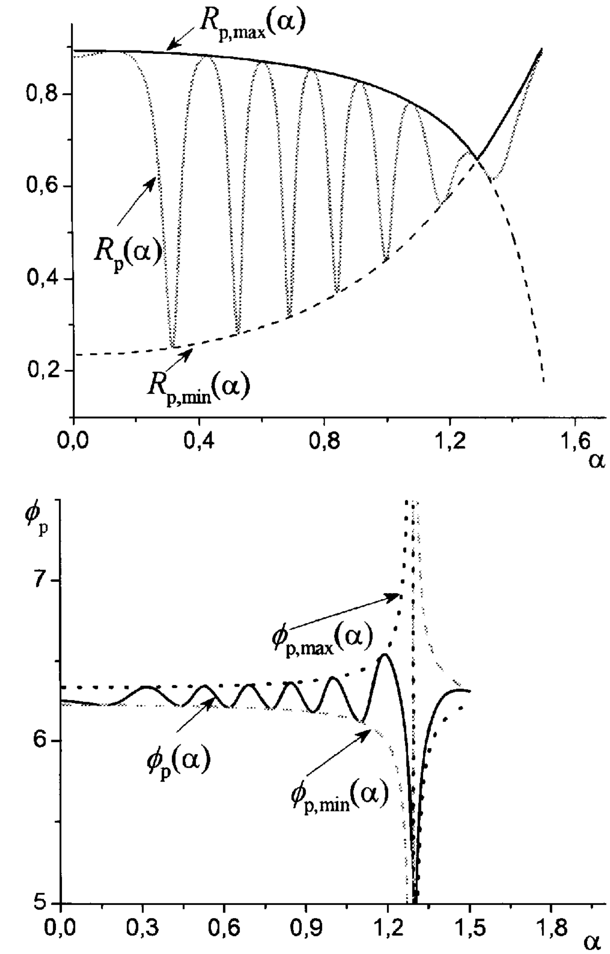


Fig. 1. Calculated amplitude-phase spectra of the oblique reflection $R(\alpha)$, $\phi(\alpha)$ and their envelope functions for the $p$-polarization; $d = 10$ $\mu$m, $\omega_0 < \omega < \omega_L$

because their values ($\alpha_{12,23}$) and the corresponding values of the energy reflection coefficients $R = |\mathrm{Re}\,\tilde{r}_{23,12}|^2$ do not depend on it [6] .

It is the angle of observation of the Brewster effect that depends on the phase thickness of the layer $\tilde{\delta}$ [10]:

$$\tilde{r}_{12} + \tilde{r}_{23} \exp\left(-i\,\tilde{\delta}\right) = 0. \quad (4)$$

The relations between the phase shifts $\phi_{12,23}$ of the waves of both polarizations for a transparent structure as the functions of the relation between the values of the refractive indices of the film and the substrate are shown in the table.

The parameters $R_{\min}$ and $b$ do not depend on $\delta$, and $b(\alpha) \neq 0$. Therefore, the Brewster effect will take place at the angles $\alpha < \alpha_{p,12} = \arcsin \frac{n}{\sqrt{1+n^2}}$ for the phase

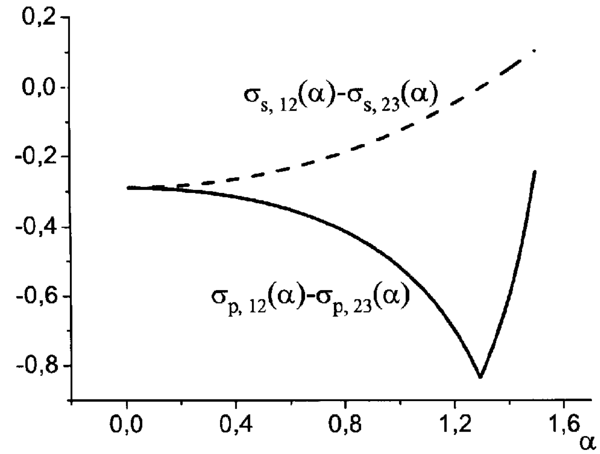


Fig. 2. Calculated curves of the angular dependence of the module difference $\sigma_{s,p,12} - \sigma_{s,p,23}$ in the range of resonant absorption of light by a substrate for the $s$- and $p$-polarizations; $\omega_0 < \omega < \omega_L$

thicknesses $\delta = \pi, 3\pi, 5\pi, \ldots$ and at the angles $\alpha > \alpha_{p,12}$ for the phase thicknesses $\delta = 2\pi, 4\pi, 6\pi, \ldots$, if the condition

$$\sigma_{12} = \sigma_{23}. \tag{5}$$

is satisfied simultaneously. For transparent structures, this condition is satisfied only in the case of $p$-polarization ($\sigma_{p,12} = \sigma_{p,23}$), with two values of the angle $\alpha$ being suitable; therefore, the equation $R_{p,\min}(\alpha) = 0$ holds true twice. Provided other relations between the structure parameters, only the Brewster quasi-effect manifests itself, and the expression for the corresponding angle expressed in terms of $\delta$ can be obtained as a solution of the equation $dR_p/d\alpha = 0$. For transparent three-layer structures and the $s$-polarization case, the inequality $\sigma_{s,12} \neq \sigma_{s,23}$ holds true for an arbitrary relation between the structure parameters and the angles, i.e. $R_{s,\min}(\alpha) > 0$ at any time. Therefore, neither the Brewster effect nor the Brewster quasi-effect can be observed for this component.

In the excitation range of an isolated excitonic resonance, which involves the spatial dispersion and the presence of an exciton-free layer on the crystal surface, the relation $R = 0$ can be realized exactly for either the $p$- or $s$-component of polarization within the exciton reflection band itself [10]. However, according to work [11], the excitonic Brewster effect or quasi-effect can be also obtained in the geometry of normal reflection at the frequency $\omega_m$, at which the compensation of a phase variation with an accuracy of $m\pi$, where $m = 0, 1, 2, 3, \ldots$, occurs; the phase variation is a result of wave propagation in the bulk of the layer and a wave reflection from the internal interface film–substrate. We recall that the spectral position of the frequency $\omega_m$ precisely traces the phase thickness of the layer, so that the value of $\omega_m$ oscillates within the limits of $\omega_0 < \omega_m < \omega_L$ as $\delta$ varies.

Although, according to general indications, the dynamics of the $\phi_{s,p,12}$ angular variations in the case of an absorbing substrate is the same as in the case of a transparent one, the condition of phase compensation

$$(\phi_{23} - \delta) = 0, \pi, .... \tag{6}$$

is significant in the resonant section of the spectrum [14].

Thus, the Brewster effect will be observed at the frequency, where both condition (6) and the equality of moduli $\sigma_{12,23}$ (Eq. (5)) will be satisfied simultaneously. The results of calculations shown in Fig. 2 testify to that the latter is obeyed only for the $s$-polarization. Therefore, if the condition of phase compensation (5) is also valid at this angle, then $R_{s,\min}(\alpha) = 0$. For the $p$- component, $\sigma_{p,12} \neq \sigma_{p,23}$ in the whole interval of the angle of incidence $\alpha$, so that $R_{p,\min}(\alpha) \neq 0$. This means that, contrary to the statement of work [10], only the Brewster quasi-effect can take place for this component.

The described features are illustrated excellently in Fig. 3. At small thicknesses of the layer (panel $a$), when $\delta(\alpha) < \phi_{23}(\alpha)$, the Brewster quasi-effect is revealed only for the $p$-polarization. As the phase thickness of the layer grows, the reflection curves for both polarizations become identical (panel $b$). If the angle, at which the phase compensation $\delta = \phi_{s,23}$ takes place, and the angle, at which the equality $\sigma_{s,12} = \sigma_{s,23}$ is fulfilled, are equal, the Brewster effect is realized. On the other hand, neither the Brewster effect nor the Brewster quasi-effect is observed for the $p$-component under the same conditions. A further growth of the phase thickness of

| | $\phi_{s,12}$ | $\phi_{s,23}$ | $\phi_{p,12}$ | $\phi_{p,23}$ | |
|---|---|---|---|---|---|
| $n < n_2$ | $\pi$ | $\pi$ | 0, if $\alpha < \alpha_{p,12}$ | 0 | $R_{s,p} = \frac{R_{s,p,\min} + b^2_{s,p}\cos^2\frac{\delta}{2}}{1 + b^2_{s,p}\cos^2\frac{\delta}{2}}$ |
| | | | $\pi$, if $\alpha > \alpha_{p,12}$ | | $R_p = \frac{R_{p,\min} + b^2_p\sin^2\frac{\delta}{2}}{1 + b^2_p\sin^2\frac{\delta}{2}}$ |
| $n > n_2$ | $\pi$ | 0 | 0, if $\alpha < \alpha_{p,12}$ | $\pi$ | $R_{s,p} = \frac{R_{s,p,\min} + b^2_{s,p}\sin^2\frac{\delta}{2}}{1 + b^2_{s,p}\sin^2\frac{\delta}{2}}$ |
| | | | $\pi$, if $\alpha > \alpha_{p,12}$ | | $R_p = \frac{R_{p,\min} + b^2_p\cos^2\frac{\delta}{2}}{1 + b^2_p\cos^2\frac{\delta}{2}}$ |

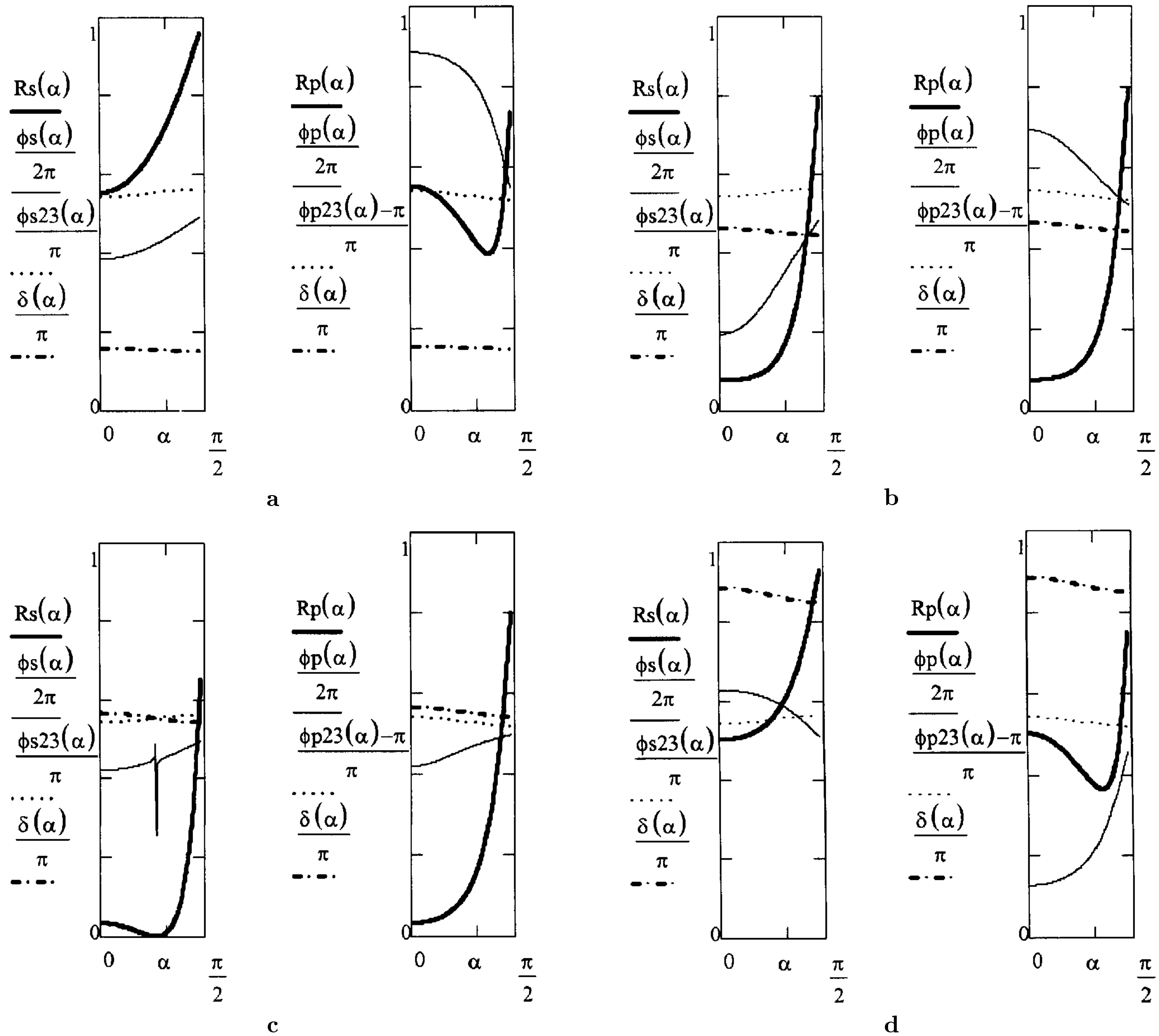


Fig. 3. Calculated curves of the reflectance, $R_{s,p}(\alpha)$, phase, $\phi_{s,p}(\alpha)$, and phase shifts, $\phi_{s,p,23}(\alpha)$, spectra of the light wave at its reflection from a film–substrate interface, and of the $\delta(\alpha)$ dependence for the wave propagation in the layers of various thickness $d = 50$ ($a$), 147 ($b$), 180 ($c$), and 280 Å($d$)

the layer results in the backward inversion of the form of the $R(\alpha)$ curve. The minimum of the latter starts to manifest itself in the $p$-polarization again (panel $d$), being absent for the $s$-component.

Let us summarize the regularities of angular variations of the amplitude-phase spectra of resonant reflection that are common and different for both polarizations. The common feature is that the values of angles, at which $r_{12} = 0$ and $\mathrm{Re}\,\tilde{r}_{23} = 0$, do not depend on $\delta$, whereas the angular position of the minimum of the curve $R(\alpha)$ does depend on it, and the condition $dR/d\alpha = 0$ is always fulfilled at those values. At the same time, the differences are as follows.

1. The curves $\delta(\alpha)$ and $\phi_{23}(\alpha)$ possess different slopes for different polarizations. For the $s$-polarization, these slopes are such that the conditions $\delta = \phi_{s,23}$ and $\sigma_{p,12} = \sigma_{p,23}$ may become true at a certain angle, and $R = 0$ exactly, although $r_{s,12} \neq 0$ at this angle. If $R > 0$ at the minimum, the corresponding angle does not equal to the angle of phase compensation.

2. The contours of the phases $\delta(\alpha)$ and $\phi_{p,23}(\alpha)$ change almost synchronously for the $p$-polarization. Therefore, there is no angle of the rigid phase compensation. For this polarization, $\phi_{p,23}$ differs from $\phi_{s,23}$ by $\pi$. Therefore, in contrast to the $s$-component, the Brewster effect is not achievable for the $p$-component as the thickness of the layer changes, and only the quasi-effect is possible.

3. The analysis of phase spectra testifies to that the multibeam interference affects the character of formation of their angular regularities in a different way. In addition to the well-known regularities, the phase $\phi_s$ is more sensitive to the Brewster transition observed in the reflection geometry (Fig. 3,$c$). In the case of $p$-polarization, the Brewster transition is accompanied only by the modification of the slope of the curve $\phi_p(\alpha)$.

That fact that the described variations of the angular spectra are caused by the multibeam interference of light in the transparent layer can be confirmed as follows. If a film with the resonant dispersion $\tilde{\varepsilon}(\omega)$ is fixed on the surface of a transparent substrate, the variations do not arise because, in this case, the Fabry—Perot effect turns out to be suppressed by the absorption effect. The phase compensation can be suppressed by increasing the damping level in the system of resonant excitations of the substrate. In this case, the angular variations are also in agreement with those resulting from the well-known Fresnel relations for the amplitudes of reflection coefficients of light from interfaces, $\tilde{r}_{s,p}$.

## 3. Conclusions

The method of envelope functions, the latter being the values of energy reflection coefficients and phases at the extrema of the Fabry—Perot interference bands, describes the angular regularities of amplitude-phase spectroscopy correctly if the light wave frequencies are beyond the range of longitudinal-transverse splitting. If the light frequency changes within the interval of a longitudinal-transverse splitting of a resonant state in the substrate medium, the Fabry—Perot interference of light in the layer and the phase variation compensation, which the wave undergoes during its propagation in the layer and at its reflection from the film–substrate interface, result in a polarization inversion of the Brewster effect. Provided that the Brewster effect is observed, the layer thickness is determined from the equation $\delta - \phi_{23} = m\pi$ and by solving the equation $dR/d\alpha = 0$ in the case of the quasi-effect.


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МОДЕЛЮВАННЯ КУТОВИХ ЗАКОНОМІРНОСТЕЙ СПЕКТРІВ ВІДБИТТЯ СВІТЛА ТРИШАРОВИМИ ПЛОСКИМИ СТРУКТУРАМИ З РЕЗОНАТОРОМ ФАБРІ—ПЕРО

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Р е з ю м е

Проведено теоретичне моделювання кутових закономірностей спектрів відбиття світла тришаровими структурами з резонатором Фабрі—Перо. Показано, що для частот світлової хвилі поза межами поздовжньо-поперечного розщеплення метод обвідних як значень енергетичних коефіцієнтів відбиття та фази в екстремумах смуг інтерференції описує ці закономірності коректно. Встановлено, що для частот світла із області поздовжньо-поперечного розщеплення можливе спостереження інверсії за поляризацією ефекта Брюстера в залежності від співвідношення між параметрами середовищ, що утворюють структуру.