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Nonlinear optimization approach to determine optical dispersion in liquid crystals

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We report the method of calculating optical dispersion of selected nematic liquid crystals using maxima positions of a transmittance filled Fabry–Pérot filter. Additionally, the profiles of a dispersive phase of reflection have been calculated. The transmittance of Fabry–Pérot filter was described as a form of a modified Airy formulae (with parameters dependence on wavelength and phase of reflection). To correctly use this function, additionally the phase of reflection is defined, taking into account the problem of a beam penetrating the mirror structure. The authors of this work assume that the point where the beam is reflected is not created strictly on the boundary of media, but it is moved into the mirror structure. The depth of the penetration changes the optical way of the wave and in consequence – the optical width of the Fabry–Pérot filter cavity. The parameter describing this phenomenon was named as a phase of reflection. This work presents how to calculate: the phase of reflection, one of refractive indices of birefringent medium inside Fabry–Pérot filter and the cavity width at the same time with the use of composed nonlinear optimization methods. The proposed method is an alternative for a reverse task solution which is hard to define properly here.

Keywords: optical dispersion, phase of reflection, liquid crystal, nonlinear optimization, Fabry–Pérot filter.

1. Introduction

The optical signal filtration by Fabry–Pérot filter (FPF) structure bases on multireflections inside an optical cavity and constructive and destructive interference phenomenon. The maximum values of transmittance have been obtained when the optical cavity width is a multiple of wavelength of an incidence wave. Then, the light beam partially confined in the cavity of FPF produces a standing wave for certain resonance frequencies. In that case, the node of the standing wave in resonance is created in the place between the mirror and the cavity of the filter, so on the boundary of media. Because the wave with energy can penetrate the medium (similar to the Goos–Hänchen effect), the real problem is included in the question: where is the real position of this last node where the wave changes the direction of propagation? In this work we assumed the following – this node is moved inside the mirror structure of the filter and its position (named here as a depth of the penetration) depends on the wavelength. Therefore, the dispersive phase of reflection can be defined as a function of d_R – the depth of the wave penetration plate in the filter and $n_R(\lambda)$ – the dispersive refractive index of the mirror in accordance with the following formula:

$$\frac{\delta_R(\lambda)}{2} = \frac{2\pi n_R(\lambda) d_R}{\lambda} \tag{1}$$

then, the real depth of the penetration mirror ("seen" by wave) is described as a coefficient $n_R d_R$.

The total change in the phase of the wave inside FPF cavity will be described as a sum of the phase change inside FPF and the phase of reflection,

$$\frac{\delta_T(\lambda)}{2} = \frac{2\pi n_{\mathrm{LC}}(\lambda) d_{\mathrm{FPF}}}{\lambda} + \frac{\delta_R(\lambda)}{2} \tag{2}$$

where d_{FPF} is the width of a Fabry–Pérot cavity.

The formulae (1) and (2) include information about the dispersive refractive index of a plate n_R and one of the refractive indices of nematic liquid crystal (NLC) n_{LC}. The NLC medium with homogenous texture has been analyzed, then n_{LC} denotes n_{o} or $n_{\mathrm{eff}} \approx n_{\mathrm{e}}$. What type of the refractive index of NLC seen by the wave depends on the orientation of linear polarizators. In the presented method we try to match the experimental values of transmittance FPF filled by NLC to the theoretical transmittance described as an Airy function with the modified total phase (see Eq. (2)) and dispersive parameters.

The refractive indices (in a visible spectrum range) of NLC can be approximated by the Cauchy formula [1, 2],

$$n_{\mathrm{LC}}(\lambda) = a_0 + \frac{a_1}{\lambda^2} + \frac{a_2}{\lambda^4} \tag{3}$$

where a_0, a_1, a_2 are the parameters which have to be calculated for each (ordinary or extraordinary) refractive index.

The quality of a change in the phase of reflection depends on the molecular structure of plates and their physical properties. In that case, a two order polynomial function (looks like the Cauchy formula) is used as well,

$$\delta_R(\lambda) = b_0 + \frac{b_1}{\lambda^2} + \frac{b_2}{\lambda^4} \tag{4}$$

A similar problem, but without the phase of reflection calculation and the optimization method description, was presented earlier in our articles [3–8].

2. Experimental setup

The presented method of calculation of refractive indices of NLC inside FPF cavity and the phase of reflection needs some information from the experiment. It is the trans-

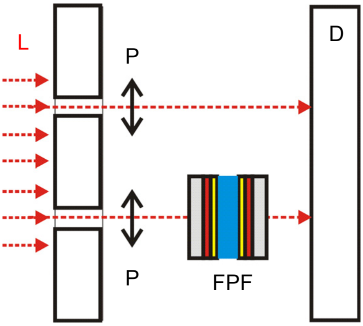

Fig. 1. Simplified scheme of a double beam Beckman spectrophotometer with FPF; L – light source (tungsten/halogen lamp), P – linear polarizers, FPF – Fabry–Pérot filter, D – detector.

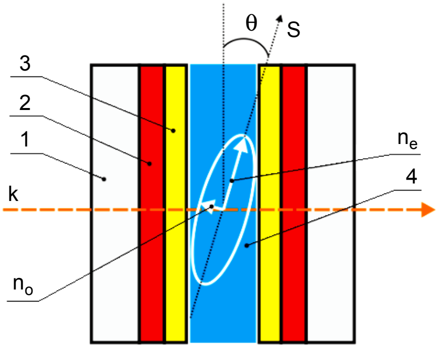

Fig. 2. Structure of plates of FPF filled by NLC with homogenous texture; 1 – glass plates, 2 – ITO electrodes, 3 – polyimide layers, 4 – liquid crystal layer, **k** – wave vector direction, *S* – director, θ – deviation angle of the director.

mittance of FPF filled by NLC measured for two different orientations of a linear polarizer corresponding to an ordinary or extraordinary wave and transmittance of the empty FPF and of the mirror (plate). The transmittance profiles were obtained using a double beam Beckman spectrophotometer. Because FPF is filled by NLC with homogenous texture – the transmittance of an ordinary wave and an effective (near extraordinary) wave is separated by two linear polarizators applied in the source and reference path of light inside the spectrophotometer (see Fig. 1). The FPF used for calculation is shown schematically in Fig. 2.

Two parallel partially transmitting mirrors, which give a reflectivity from 60% to 67% covered with 50 nm transparent indium-tin-oxide (ITO) layers are used to construct the plates of a filter. The profile of the reflectance of mirrors (both were the same in experiment) is shown in Fig. 3. Plates were separated by means of glass spacers with the diameter from 6 to 10 μm.

The refractive index for an extraordinary wave n_e was calculated from the following relationship:

$$n_{\mathrm{eff}}(\theta, n_o, n_e) = \frac{n_o n_e}{\sqrt{n_o^2 \cos^2(\theta) + n_e^2 \sin^2(\theta)}} \tag{5}$$

The angle θ denotes an angle between the plane parallel to the plate and the optical axis in the NLC layer.

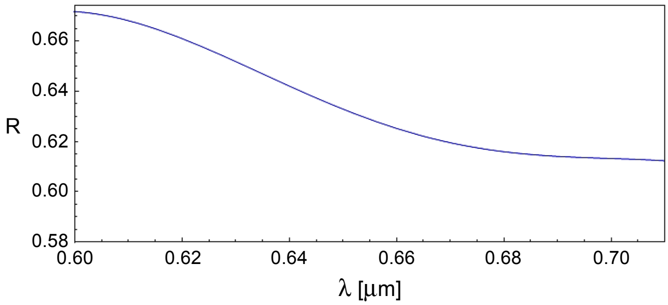

Fig. 3. The profile of mirror reflectance used for calculation.

After the experiment, all information – the transmittance (for a visible range) of a filled FPF for ordinary and effective waves, the transmittance of the mirror and the transmittance of an empty FPF – have been prepared for optimization. Those data were applied as starting data for the nonlinear optimization method.

3. Method of calculation using optimization

To calculate discrete data $(n_{\mathrm{o}}^{i}(\lambda), n_{\mathrm{e}}^{i}(\lambda))$ for approximation profiles of refractive indices of NLC $(n_{\mathrm{o}}(\lambda), n_{\mathrm{e}}(\lambda))$, the filter transmittance for the selected state of polarization and the dispersive refractive index profile of FPF plate $(n_R(\lambda))$ calculated based on the profile of reflectance (see Fig. 1) are needed. The distance between interference peaks (see Fig. 4) increases along, where the wavelength is escalated. This feature is used to perfectly fit the experimental peak positions to the theoretical peak positions. The theoretical peak positions were obtained as a result of the theoretical transmittance analysis. The peak positions agreement is possible when using the function of the total phase (Eq. (2)) which includes information about the phase of reflection.

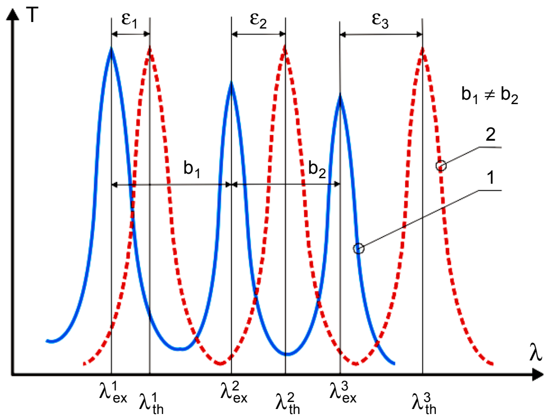

Fig. 4. Positions of interference maxima from experimental transmittance for three peaks (curve 1) and position of theoretical peaks of transmittance (curve 2); ε denotes distance between the maxima of theoretical and experimental transmittance.

The problem of the distance minimization between the experimental peak positions λ^i_{ex} and the same obtained from theoretical transmittance λ^i_{th} is possible to describe as an objective function for i-analyzed peak of transmittance:

$$F(\lambda^i_{\mathrm{ex}}, n_{\mathrm{LC}}, n_R, d_{\mathrm{FPF}}, \delta_R) = \sum_i \Big[\varepsilon(\lambda^i_{\mathrm{ex}}, n_{\mathrm{LC}}, n_R, d_{\mathrm{FPF}}, \delta_R)\Big]^2 =$$

$$= \sum_i \Big[\lambda^i_{\mathrm{ex}} - \lambda^i_{\mathrm{th}}(n_{\mathrm{LC}}, n_R, d_{\mathrm{FPF}}, \delta_R)\Big]^2 \tag{6}$$

The theoretical peak positions λ^i_{th} were obtained from the formula describing the transmittance of FPF (Eq. (7)) modified using Eqs. (1), (2) and also with the use of conditions formulated by Eqs. (11)–(14). It is very hard to say which one responds to those obtained from the experiment. Additionally, n_{LC} and δ_R values needed for a full description of the theoretical transmittance Eq. (7) [9, 10] are not known. It is possible to restrict its behavior with properly constructed nodes. So, the task for the optimization procedure is denoted as below:

$$T_{\mathrm{th}}(\lambda) = \left\{\frac{1-4R(\lambda)}{[1-4R(\lambda)]^2\sin^2(\delta_R/2)}\right\}^{-1} \tag{7}$$

$$R(\lambda) = \left[\frac{n_{\mathrm{LC}}(\lambda) - n_R(\lambda)}{n_{\mathrm{LC}}(\lambda) + n_R(\lambda)}\right]^2 \tag{8}$$

$$\left.\frac{\mathrm{d}T_{\mathrm{th}}(\lambda)}{\mathrm{d}\lambda}\right|_{\lambda = \lambda^i_{\mathrm{th}}} = 0 \tag{9}$$

To calculate the profile of the refractive index and the phase of reflection of NLC at the same time, we have to establish the objective function as

$$F(n^*_{\mathrm{LC}}, d^*_{\mathrm{FPF}}, \delta^*_R, \lambda^{i*}_{\mathrm{ex}}) = \min[F(\lambda^i_{\mathrm{ex}}, n_{\mathrm{LC}}, n_R, d_{\mathrm{FPF}}, \delta_R)] \tag{10}$$

and the boundary conditions for all parameters:

$$n_{0\mathrm{LC}} \le n_{\mathrm{LC}} \le n_{1\mathrm{LC}} \tag{11}$$

$$d_0 \le d_{\mathrm{FPF}} \le d_k \tag{12}$$

$$\delta_0 \le \delta_R \le \delta_k \tag{13}$$

$$\lambda^i_{\mathrm{rel}} - \Delta\lambda \le \lambda^i_{\mathrm{ex}} \le \lambda^i_{\mathrm{rel}} + \Delta\lambda \tag{14}$$

where: d_0, d_k, δ_0, δ_k, $n_{0\mathrm{LC}}$, $n_{1\mathrm{LC}}$, $\Delta\lambda$ are scalar values; values with index i are values for i-peak of transmittance.

It is a very important problem for the optimization method, so the formula (2) includes two conjugated variables (n_{LC} and d_{FPF}) to calculate. There are no numerical methods to do it properly. Thus, the procedure of optimization can be applied several times for different values of d_{FPF} (changed from the range of d_0 to d_k with step Δd). The process of optimization starts for d_{FPF} equal to d_0. The vector of start parameters $\{n_{0\mathrm{LC}}, n_{1\mathrm{LC}}, d_0, d_k, \delta_0, \delta_k\}$ is given from the basic knowledge about the material (nematic liquid crystals) and the properties of the Fabry–Pérot construction; the deviations $(\lambda^i_{\mathrm{rel}} \pm \Delta\lambda)$ are a consequence of measurement errors of peak positions. For a given value of d_{FPF} and selected λ^i_{ex} (i-experimental peek position) with a measurement error $\Delta\lambda$, it is possible to obtain a set of pairs $\{n_{\mathrm{LC}}, \Delta R\}_i$ by minimization of the objective function (10). This procedure will be repeated for all analyzed peaks. From that set, only one pair of data $\{n_{\mathrm{LC}}, \delta_R\}$ for one peak position is selected, based on the criteria below:

i) decreasing trend of discrete refractive indices values for all analyzed peaks (if it is possible),

ii) $\|\lambda_{\mathrm{ex}} - \lambda_{\mathrm{th}}\|_2 = \min$, for pair $\{n_{\mathrm{LC}}, \delta_R\}$,

iii) $\sum_{i=1}^{n-1} \left|\delta_T^{i+1} - \delta_T^i\right| \le n\pi$, phases for all analyzed peaks (n-peaks).

The process is completed for one value of d_{FPF}. The analysis will be repeated for next d_{FPF} values. From the set of the results, this one which assures the best fit transmittance to the experimental peaks position is approved.

The discrete result of each refractive index (ordinary and effective) of NLC and the phase of reflections was approximated by a polynomial function (Eq. (3) or (4)), adequately. This approximation can increase the error between the peaks position of T_{th} and the peaks position of T_{ex}. Therefore, the approximation procedure is a part of the optimization task. In literature it is not strictly described how to approximate the discrete values of the phase of reflection. The authors propose that the approximation should look like the Cauchy form, but the phase of reflection may change values between the discrete values and the modified approximation result considerably. The differences between the results of the phase of reflection for each other media are a consequence of different depth of the plate penetration by waves with different wavelengths.

4. Results for 5CB and 1292 nematic liquid crystalline media

The results of calculation (Figs. 5–12) are shown for two different NLCs media – well known and widely described in literature 5CB (4-cyano-4′-pentylbiphenyl) and the liquid crystalline nematic mixture 1292 (from the laboratory of prof. Dąbrowski from Military University of Technology, Department of Chemistry, Poland). All curves of refractive indices are monotonically decreasing in accordance with expectations. All points on the figures below present the calculated values. Their positions (on the λ-axis) correspond to the positions of transmittance maxima obtained from the experiment. The approximation values are shown in the form of the solid lines.

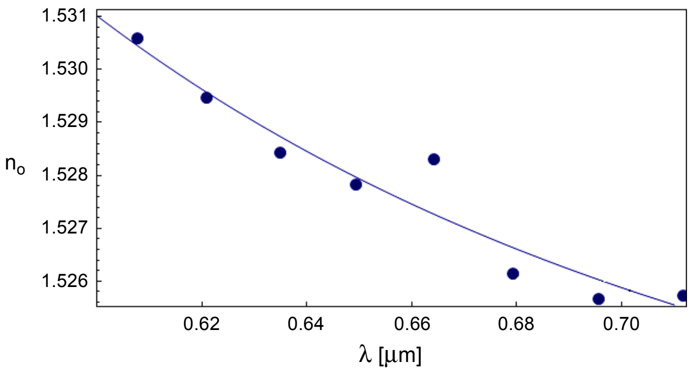

Fig. 5. Profile of ordinary refractive index for 5CB.

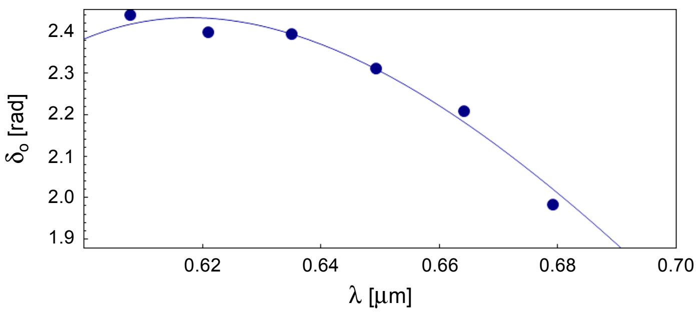

Fig. 6. Profile of phase of reflection for ordinary waves, and for FPF filled by 5CB (variant).

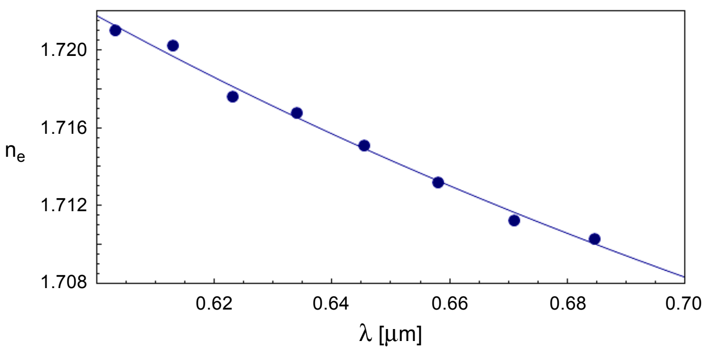

Fig. 7. Profile of extraordinary refractive index for 5CB.

The values of coefficients of approximation polynomials (Eqs. (3) and (4)) are given in Table 1. This Table includes information about calculated optical cavity width of filled FPF.

The decreased profile of refractive indices of liquid crystalline agrees with the theory of the optical dispersion of materials for a visible spectrum range. The decreased phase of reflection, in that case, denotes the different depth of the penetration wave.

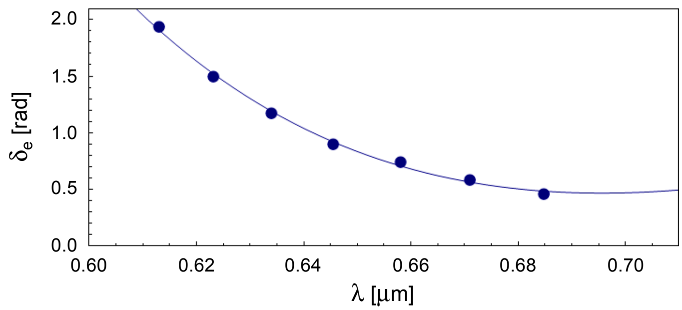

Fig. 8. Profile of phase of reflection for FPF filled by 5CB, and extraordinary wave (variant).

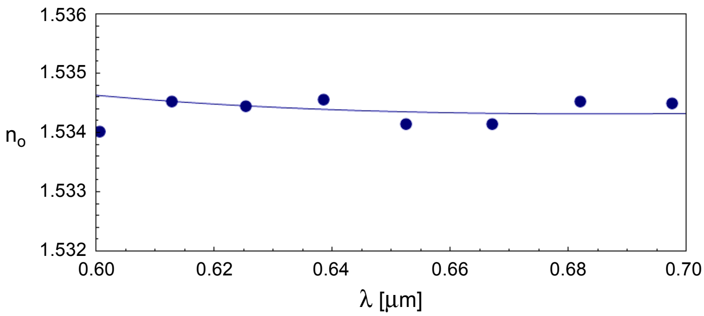

Fig. 9. Profile of ordinary refractive index for 1292.

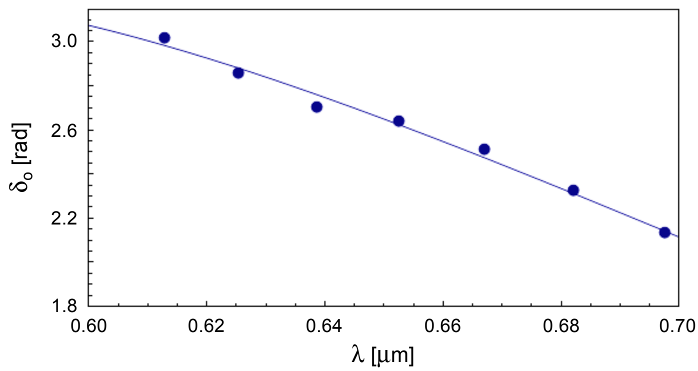

Fig. 10. Profile of phase of reflection for ordinary waves, and for FPF filled by 1292 (variant).

Precisely, it is the difference between the LC layer and the plate boundary and the first wave node inside the plate structure. Thus, the wave of short wavelength and higher energy penetrates more than longer waves. For two differently oriented linear polarizations and one construction, two different profiles of the phase of reflection have been obtained in this work. How is it possible? It is not only a numerical result. The coefficient of reflection on the boundary of two media is different for two perpendicular

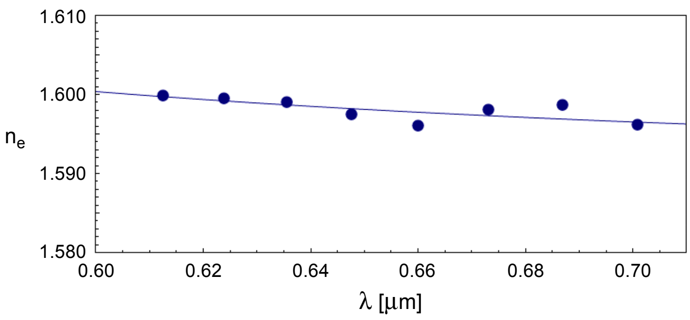

Fig. 11. Profile of extraordinary refractive index for 1292.

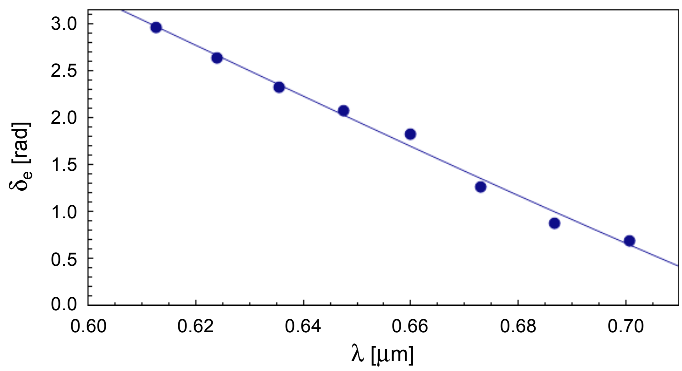

Fig. 12. Profile of phase of reflection for FPF filled by 1292, and extraordinary waves (variant).

T a b l e 1. Results of calculation of refractive indices and phases of reflection.

NLC	Refractive index	Refractive indices*			Phase of reflection*			Cavity width
		a_0	a_1	a_2	b_0	b_1	b_2	d [µm]
5CB	n_o	+1.52078	+0.00161	–0.00079	–11.5345	+10.6690	–2.03727	8.9800
	n_e	+1.66866	–0.00043	+0.02032	17.9172	–16.8874	+4.08523	
1292	n_o	+1.53779	–0.00325	+0.00076	–5.21304	+5.27097	–0.82360	9.3910
	n_e	+1.59049	+0.00130	+0.00081	–12.30070	+8.40024	–1.00380	

*Coefficients values of approximate polynomial.

linear polarizations, because two different refractive index values for one medium (NLC) were found. Thus, the coefficient of reflection depends on linear polarizer orientation and then the phases of reflection may be different.

5. Conclusions

The calculation of optical dispersion of refractive indices and the phase of reflection for all observed waves at the same time offers a new quality for building Fabry–Pérot optical filters. Using those results, one can observe and correct parameters values of a filter working in different weather and experimental conditions. Such method will be useful for another part of spectrum as well. Results are shown for FPF with dielectric plates only. The phase of reflection on the boundary LC/dielectric plates includes information about the depth of penetration into plates. The decreased penetration of longer waves into dielectric plates and, inversely, the growing penetration for shorter waves (as a consequence of Eq. (1), where d_R is defined) has been observed. The optimization task seems to be much more effective than the reverse task to obtain coefficients in Cauchy polynomials. The reverse task is really hard to be properly defined here.

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