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INFLUENCE OF LOW-PASS FILTER PARAMETERS ON DECONVOLUTION OF SPECTRAL BANDS

D. K. Buslov, N. A. Nikonenko,
and R. G. Zhbankov

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One of the most important problems in interpreting the spectra of complex substances is the substantial overlap of neighboring wide absorption bands, which causes insufficient resolution of them. Among the various methods of separation of individual components in a complex spectrum are linear methods of mathematical peaking of spectral bands and, in particular, the deconvolution method [1]. However, peaking the initial bands in this method is accompanied, as a rule, by a change in the initial shape of the spectral contour. In some cases extra peaks of a different amplitude may be formed even in the absence of random errors, which complicates substantially the extraction of information on the number and positions of separate components in a complex spectrum.

As was shown earlier [2], the transfer function in the deconvolution method is a sum of the transfer functions of high- and low-pass filters. If the transfer function of a high-pass filter matches the shape of the initial band, then the initial shape of the contour may change only owing to a low-pass filter (LPE) [3]. The larger the band peaking is required, the stronger the LPF effect. In the case of self-deconvolution the shape of the resultant band is described by the pulse response of the LPF, i.e., it is completely determined by the filter parameters, namely, its cut-off frequency β and the transition band width δ. The LPF transmission band with a symmetrical transition band is $\Omega_2 = \beta+\delta/2$. Given the transmission band, a change in δ inevitably entails a change in β. Therefore it is necessary to consider the simultaneous change of these parameters, which is conveniently described by $\kappa = \delta/2\beta$.

In [4], the maximum oscillation amplitudes of the resultant contour are given for different apodization functions in the case of self-deconvolution. However, for optimization of the deconvolution parameters the distribution of the oscillation amplitudes with increase in distance from the principal maximum and their dependence on the LPF parameters are important. This problem may be solved using the analytical expression for the resultant contour obtained in [3] for a spectral band of dispersion form.

If band narrowing is at its maximum (the half-width of deconvolution is close to that of the initial band), the expression for the shape of the resultant contour becomes

$$S(x)=\frac{Z_0W_0}{2}\Big\{\beta\cos(\delta x/2)\,\mathrm{sinc}(\beta x)+\frac{\delta}{4}\sin(\beta x)\,\mathrm{sinc}(\delta x_1/2)+ \\ +\frac{\delta}{4}\sin(-\beta x)\,\mathrm{sinc}(\delta x_2/2)\Big\}, \tag{1}$$

where Z_0, W_0 are the amplitude and the half-width of the initial band, respectively; $x_1 = \pi/\delta - x$; $x_2 = \pi/\delta + x$. From (1) it follows that the contour of the band $S(x)$ in the general case is a result of the superposition of three oscillating components, the principal maximum of one of which coincides with the maximum of the initial band, while the principal maxima of the other two are symmetrical to the central one. As a consequence, oscillations whose frequency and amplitude depend strongly on the LPF parameters used may occur in the resultant contour.

We now consider the influence of the choice of the low-pass digital filter parameters on the effectiveness of the oscillation compensation process. For this, by analogy with [4] we introduce the relative amplitude of the extra peaks of the resultant contour

$$S_k=S(x_k)/S(0), \tag{2}$$

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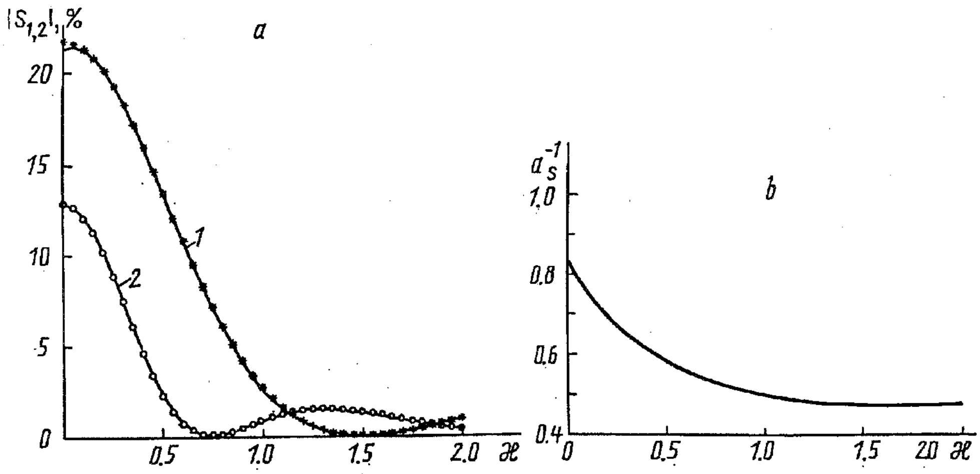

Fig. 1. Absolute values of the relative amplitude of the first (1) and second (2) extra peaks (a) and the shape parameter a_s (b) versus κ.

where $S(0)$, $S(x_k)$ are the amplitudes of the principal and k-th extra peaks, respectively. The problem of determination of the oscillation amplitudes $S(x_k)$ of the curve obtained is reduced to determination of the extrema of the function $S(x)$. Since the resultant contour is described by the rather complicated expression (1), having transcendental functions, the equation for the extrema of the function $S(x)$ is solved numerically in the general case.

In the case of self-deconvolution, the relative oscillation amplitudes S_k of the resultant contour may be described by the approximate formulas

$$S_k \approx \begin{cases} \dfrac{(-1)^k 2(1+\varkappa)^3 \sin[\pi/(2(1+\varkappa))]\cos[\pi\varkappa/(2(1+\varkappa))+\varkappa\pi k]}{\pi[2k(1+\varkappa)+1][(1+\varkappa)^2-\varkappa^2(2k(1+\varkappa)+1)^2]}, \\ \qquad 0\leqslant\varkappa\leqslant\varkappa_k, \\ \dfrac{2(1+\varkappa)^3\sin[(2k+3)\pi/(2(1+\varkappa))]\cos[(2k+3)\pi\varkappa/(2(1+\varkappa))]}{\pi(2k+3)[(1+\varkappa)^2-\varkappa^2(2k+3)^2]}, \\ \qquad \varkappa_k\leqslant\varkappa\leqslant 2, \end{cases} \tag{3}$$

where $k = 1-m$; $\kappa = \delta/2\beta$; $\kappa_k \cong \begin{cases} 1 \text{ for } k=1, \\ 0.5 \text{ for } k>1. \end{cases}$

As seen from (3), the relative amplitudes of the extra peaks of the resultant curve are fully determined by κ, i.e., by the ratio of β and δ. At $\kappa = 0$ (the ideal LPF) oscillations of the contour obtained damp slowly as k increases according to a 1/k law:

$$S_k \approx \frac{(-1)^k 2}{\pi(2k+1)}.$$

Using this relation, it is easy to show that only at k~30 does the value of the relative amplitude of the extra peaks decrease to 1%. The condition $\kappa = 1$ ($\delta = 2\beta$) provides smooth decrease of S_k in conformity with the approximate relationship

$$S_k \approx \frac{(-1)^k 8}{\pi(2k+1)(2k+3)(2k+5)}.$$

As is seen, the amplitude of the k-th extra peak undergoes a $(k+2)^2$-fold decrease as compared to the ideal LPF. As a result, the amplitudes of all the extra peaks, starting from the second peak, make up less than 1% of the amplitude of the principal peak. Thus, analysis of the expression for the relative oscillation amplitudes of the resultant contour shows that the larger the magnitude κ of the ratio of β and δ of the LPF, the more rapidly these amplitudes die down.

TABLE 1. Half-Width of the Resultant Contour W_s and Displacement of Side Components d as a Function of κ

κ	0.25	0.50	0.75	1.0	1.25	1.50	1.75	2.0
W_s	3.80	4.30	4.72	5.00	5.16	5.22	5.22	5.22
d	1.65	2.0	2.30	2.50	2.60	2.70	2.70	2.70
$2d/W_s$	0.87	0.93	0.97	1.00	1.01	1.03	1.03	1.03

Note: $\Omega_2 = 0.4$.

The dynamics of the change of the largest amplitudes of the first $|S_1|$ and the second $|S_1|$ extra peaks with on the parameter κ is shown in Fig. 1a. It is seen that S_1 and S_2 calculated by approximate formulas (3) almost coincide with the experimental relative amplitudes of the extra peaks. Hence it follows (Fig. 1a) that by changing the ratio transition bandwidth to the cut-off frequency of the filter we may vary the oscillation amplitude of the resultant contour. The oscillation frequency of the spectral curve obtained depends on the absolute values of the above LPF parameters.

Changing κ is equivalent to replacing the apodization function, which, as is known [4], entails a change of a half-width of the curve obtained. Using expression (1) for S(x) we can show that the half-width W_s of the resultant contour as a function of β and δ of the LPF may be described by the transcendental equation

$$4\sin(\beta W_s/2)\cos(\delta W_s/4) - (\beta W_s)\left[1-(\delta W_s/2\pi)^2\right] = 0. \tag{4}$$

Solutions of Eq. (4) for different β-to-δ ratios of the LPF (Ω_2 = const) are given in Table 1. For comparison purposes Table 1 also lists displacements d of the principal maxima of the side components of the resultant contour S(x) of (1). The relative quntity $\Delta = 2d/W_s$ in the transition bandwidth range $\delta \geq 2\beta$ is seen to be practically unchanged and equal to unity. This is indicative of the important role of the two last summands in (1) in forming the half-width of the resultant contour. Deviations of Δ from unity are observed only when the transition bandwidth approaches zero, i.e., when the half-width of the curve obtained becomes identically equal to that of the central component. From Table 1 it also follows that for a given boundary of the transition band Ω_2 an increase in κ makes the principal maxima of the side components depart from the central maximum, thus broadening the resultant contour.

By analogy with [4] we present the half-width of the contour obtained under self-deconvolution conditions in the form $W_s = \pi a_s/\Omega_2$, where a_s is a shape parameter, whose value is specified for a given apodization function. In this case, the two-parameter equation (4) passes into the one-parameter equation

$$4(1+\varkappa)\sin[\pi a_s/2(1+\varkappa)]\cos[\pi a_s\varkappa/2(1+\varkappa)] - \pi a_s\left[1-a_s^2\varkappa^2/(1+\varkappa)^2\right] = 0, \tag{5}$$

whence it follows that the shape parameter a_s, just like the relative amplitude S_k of the extra peaks, is a function of the ratio κ of the LPF parameters β and δ (Fig. 1b). This means that by varying κ one may gradually change the parameter a_s by decreasing or increasing the half-width of the resultant contour W_s. In this case the boundary of the transition band Ω_2 remains unchanged. The degree of mathematical accentuation of the initial band, specified by the parameter $K = W_0/W_s = W_0\Omega_2/\pi a_s$, is inversely proportional to a_s. Therefore the decrease in the shape parameter a_s with decrease in the ratio κ is accompanied by an increase in the degree of peaking of the initial band.

A comparison of the plots of $|S_{1,2}|$ and a_s^{-1} versus κ (Fig. 1) shows that by varying the parameter κ one may change the relationship between the degree of mathematical peaking of the initial band for a given Ω_2 and the obtained shape of the spectral contour. In this case the decrease in the amplitude of the extra peaks with increase in κ is accompanied by a decrease in the degree of peaking of the initial band and vice versa.

Optimization of the ratio of the LPF parameters depends on the requirements specified for the half-width and shape of the spectral contour produced by deconvolution. In many cases in order to separate individual components in a complex spectrum it is necessary to provide maximum peaking of the initial bands. The most general

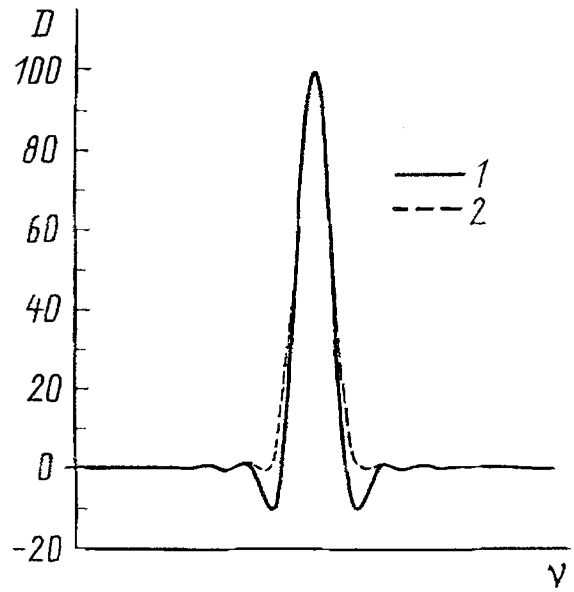

Fig. 2. Results produced by a digital self-deconvolution filter at $\kappa = 0.6$ (1) and 1.7 (2).

requirement on the shape of the resultant contour is the absence of extra maxima, which create the greatest difficulties in interpreting the obtained results of mathematical processing.

Let the constraints imposed on the half-width and shape of the resultant curve be expressed in terms of the relative amplitude of the extra peaks S_k and the shape parameter a_s. Then the optimization criterion may be written in the form

$$\begin{cases} |S_k(\varkappa_0)| \leqslant n\ \%, \\ a_s(\varkappa_0) = \inf a_s(\varkappa), \end{cases} \tag{6}$$

where n is the permissible value of the relative oscillation amplitude. The problem of determining the value κ_0 satisfying criterion (6) is solved numerically using the relations for $S_k(\kappa)$ and $a_s(\kappa)$. For instance, the curves in Fig. 1 show that for n = 1 and k>1 the first condition of criterion (6) is satisfied by κ in the intervals $0.6 \leq \kappa \leq 1$ and $1.7 \leq \kappa \leq 2$. The second requirement of attaining the minimum value of a_s is fulfilled at the smallest value of κ, i.e., at $\kappa_0 \approx 0.6$. In the given example the optimal ratio of the transition bandwidth to the double cut-off frequency of the filter is approximately 0.6. In this case for a given boundary of the transition band Ω_2 the greatest possible degree of peaking of the initial band is attained, while the resultant contour shows virtually no extra maxima (Fig. 2, curve 1). At the same time, as follows from the figure, for the given ratio of the LPF parameters there are two negative peaks on the spectral curve obtained that are symmetric relative to the principal maximum. The relative amplitude of these peaks is approximately 11%.

Under certain conditions of overlap of separate bands the presence of negative peaks on the contour produced by deconvolution may be undesirable. In order to obtain a shape of the resultant curve identical to the initial one, it is necessary to impose a more rigorous, as compared to the previous condition, limitation on the relative amplitude of the extra peaks, namely, n = k = 1. As is seen in Fig. 1a, the first condition of criterion (6) in this case is satisfied by the parameter κ in the interval $1.7 \leq \kappa \leq 2$. As follows from Fig. 1b and Table 1, in this range of the ratio of the LPF parameters the shape parameter a_s is practically independent of κ. It may be concluded that choosing the ratio of the transition bandwidth to the double cut-off frequency of the filter in the interval $1.7 \leq \kappa \leq 2$ ensures obtaining the simplest form of the resultant contour. However, the degree of peaking of the initial band for a given boundary value of the transition band Ω_2 is somewhat smaller than in the previous case (Fig. 2, curve 2).

The performed analysis of the influence of the choice of low-pass digital filter parameters on self-deconvolution of spectral bands reveals that the values of the relative amplitude of the extra peaks of the curve obtained as well as of the shape parameter are determined by the ratio of the transition bandwidth to the cut-off frequency of the low-pass filter. The choice of the optimal ratio of the above filter parameters depends on the trade-off between the required degree of mathematical peaking of the initial band, on the one hand, and the obtained form of the spectral contour, on the other. In conclusion, we note that when apodization functions are approximated by concrete digital filters, the values of the oscillation amplitudes of the resultant curve may differ somewhat from the analytical values considered.

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