THE ALGORITHM AND PROGRAM FOR PROCESSING LINEAR SPECTRA

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We present the algorithm, which allows to process linear spectra containing overlapped peaks. The program using this algorithm provides a fast processing procedure for any linear spectra at arbitrary radiation background conditions.

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It is in common usage to process linear spectra by using different fitting functions, as a rule one makes a use a Gauss function or some linear combination of such functions[1]. At this it is assumed that dispersions of single peak does not depend on its positions in a spectrum [2]. Such approach, in our mind, can result in loss of information concerning physical nature of processes that result in occurrence of radiation peaks. As an illustration of this situation one can see the spectra of coherent X-ray radiation (CXR) in [3, 4]. In these spectra the observable radiation lines are characterized by asymmetry of their form and, moreover, their linewidths depend essentially on positions which the weight centers of these lines have on an energy scale [4].

We elaborated the algorithm and program package for processing linear spectra, which is free from the above lacks. This processing algorithm executes the following steps:

1) Construction of a reduced spectrum S' by making a convolution procedure. At this an initial spectrum S is convoluted with a correlator K which has a width k and zero area:

$$S'(j) = \sum_{i=j-3k}^{j+3k} S(i)K(i),$$

where j is the channel number and $\sum_{i=j-3k}^{j+3k} K(i) \equiv 0$.

2) Definition of non-zero areas in the reduced spectrum and identification of weight centers of these areas with weight centers of peaks in the initial spectrum.

3) Generation for each peak p in S' a Gauss-like peak $G(\sigma_p, h_p)$ having dispersion σ_p and height h_p. Construction of a reduced Gaussian spectrum by convolution with K:

$$G'(j) = \sum_{i=j-3k}^{j+3k} G(\sigma_p, h_p; i)K(i).$$

At this stage the initial values for peak dispersions are assumed to be equal for all peaks in the spectrum and equal to a value of dispersion in a calibration spectrum obtained by using standard radioactive sources.

4) Minimization of function $(G'-S')^2$ for each peak p with respect to the parameters σ_p and h_p by the Newton's method (see, for example, [5]). Minimization procedure is fulfilled for three points, which are at the edges and in the weight center of the peak non-zero area found on the step 2.

5) Values σ_p and h_p found on the step 4 are taken as *previous* characteristics of the peaks and used for definition of 3σ-limits in S. If the boundaries of neighbor peaks are overlapped then peak groups are formed. Then these peaks are copied to separate buffer spectra and common boundaries of these buffers are marked.

6) Subtraction of a background from S. When this procedure is performed the background under peak and/or peak groups is approximated by the linear function and written to the separate buffer spectrum F.

7) Area of overlapping for peak groups is fixed. In this region the peaks are approximated by a Gauss function with σ_p and h_p found on the step 4. Deconvolution of peaks in the overlapping areas is made as it is described in [2].

8) Definition of sums A_p under peaks, positions X_p of weight centers and dispersions Δ_p in the initial spectrum.

9) Definition of the statistical importance of found peaks by a criterion $A_p > F_p^{1/2}$, where F_p is the sum of background counts under peak p which is calculated by using the background buffer spectrum F defined on the step 6. If such peak does not satisfy to this criterion then it is erased from the initial spectrum. In the case when this peak was marked as a member of a peak group then the steps 1-7 are repeated for this part of the initial spectrum.

10) Calculation of statistical errors connected with definition of A_p, X_p and Δ_p.

As we said above, the most acceptable magnitude of k is equal to a value of dispersion of calibration peaks. Note that the algorithm will work in that case when calibration data are absent at all. In this case the initial value of k can be set arbitrary and on the step 4 that values of dispersions σ_p will be found which minimizes the function $(G'-S')^2$. If one takes into account that values of peak dispersions found on the step 4 are used only as intermediate results, and the true values are defined on the step 8, it is possible to tell that the processing of spectra by the algorithm described does not require special calibration measurements.

The program developed was used for processing spectral data obtained in investigating the CXR's properties during the run period at the 40-MeV linear electron accelerator LUE-40 (NSC KIPT). In these measurements we used a 5-mm thick Si(Li) solid-state detector having energy resolution of 350 eV for

13.7 keV line of a source ^{241}Am. Fig. 1 shows three radiation spectra, which were obtained during the experiments with a 54 μm thick germanium crystal [4]. These spectra demonstrate the features of work of the processing program.

In Fig. 1,a the CXR peak and the K_α peak of ^{44}Ru, which is an admixture element for the crystal used, are placed as the isolated ones. Fig. 1,b illustrates that situation when the peak group is fixed on the step 5. In Fig. 1,c CXR peak covers the K_α peak completely. In this case the peak is processed as an isolated one and to define its A, X, Δ and statistical errors connected with these values the data for K_α peak obtained from spectra like 1b are used. Fig. 2 shows the results of processing for series of CXR spectra. This figure demonstrates the dependence of CXR linewidths on position of the weight centers on the energy scale.

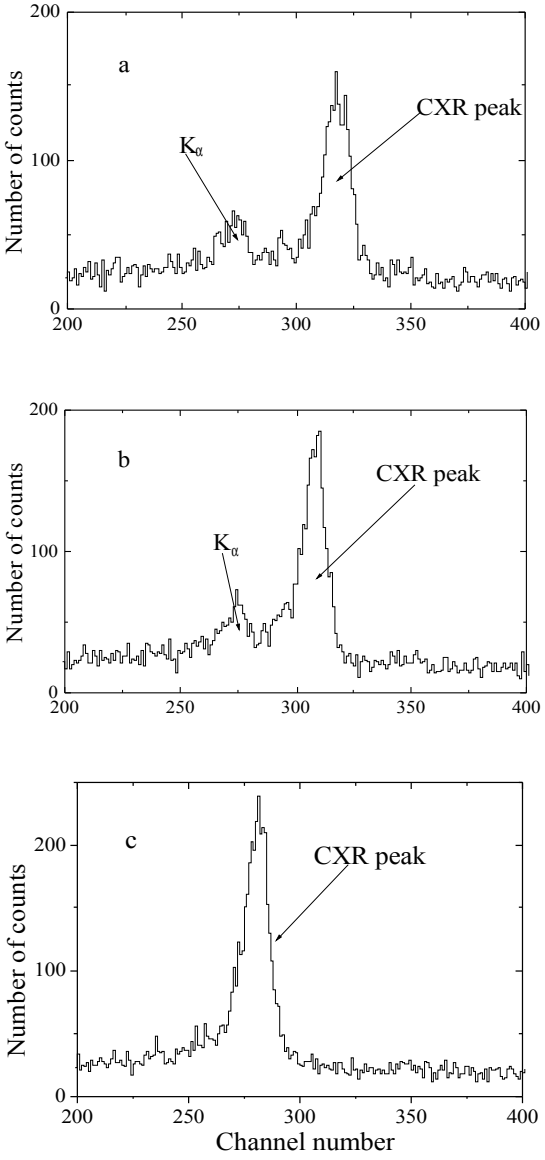

Fig. 1. *The series of CXR's spectra demonstrates the different variants of processing: (a) - two isolated peaks; (b) – peak group; (c) – complete covering*

The investigation carried out shows a high reliability and productivity of the processing algorithm. It should be noted that execution of step 4 requires not more than 10 iterations even if initial values of σ_p and h_p were chosen far from the real ones. The program was written using Visual Basic 5.0, the target system is Windows 9x/NT.

The program has a convenient and understandable user interface, which allows make changes of the processing parameters easily. The program prints on the screen and writes to a file the processing results and it gives the information about the place and conditions at which the spectrum was obtained.

There are several data formats, which are supported by the program. These data can be presented as a continuous table, which contains only count numbers, or as the table, which contains channel numbers and count numbers as well.

The evaluation version of the program is distributed freely by the request.

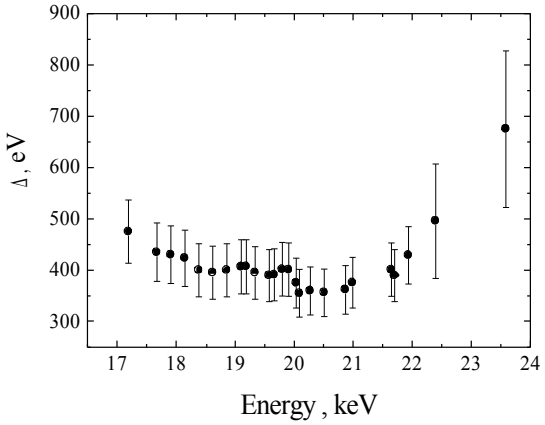

Fig. 2. *Dependence of CXR peak dispersion on energy as it was determined by processing the series of spectral data*

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