A Parametric Formulation of the Resolution Function of a Pulsed-source Chopper Spectrometer

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Abstract

Based on a previously developed formulation for the resolution function of a pulsed-source chopper spectrometer, we describe an algorithm which facilitates the application of resolution calculations in data analysis. The method consists of an estimate of the source pulse shape parameters from a least-squares analysis of the monitor spectra and an efficient evaluation of the spectrometer resolution functions over a wide range of energy transfers using a parametric expression.

I. Introduction

The source pulse emission time distribution (pulse shape) bears important consequences in the energy-scale calibration and the characterization of the resolution function of a pulsed-source chopper spectrometer, of which the major components are shown schematically in Fig. 1 (see also Table I). The choppers transmit a narrow energy-band of neutrons of which the velocity distribution is not symmetric with respect to the mean velocity. As the neutrons travel along the flight path, they spread out in time, resulting in progressively skew intensity profiles, as shown in the beam monitor spectra (panels 1b and 1c). The intensity of the scattered neutron beam at a detector exhibits a similar skew time-of-flight profile that varies with the neutron energy-transfer E, as shown in panel 1d. In 1987 we demonstrated[1] how the resolution function of a pulsed-source chopper spectrometer could be calculated through an analysis of the neutron intensity distribution, $I_s(v,t)$, as a function of the neutron speed (v) and flight time (t). It involves an evaluation of a convolution integral of the source spectrum and pulse shape with the response functions of all the relevant components (moderator, choppers, collimators, detectors, etc.) of the spectrometer. The agreement between calculated and observed spectra at various configurations was borne out by experiments.

Two problems arise in the application of the resolution calculations in routine data analyses: 1) the parameters of the Ikeda-Carpenter pulse-shape function[2] under the target-moderator conditions during the experiments are usually not available; and 2) the rather long computer time required for the evaluation of the resolution functions over the measured energy

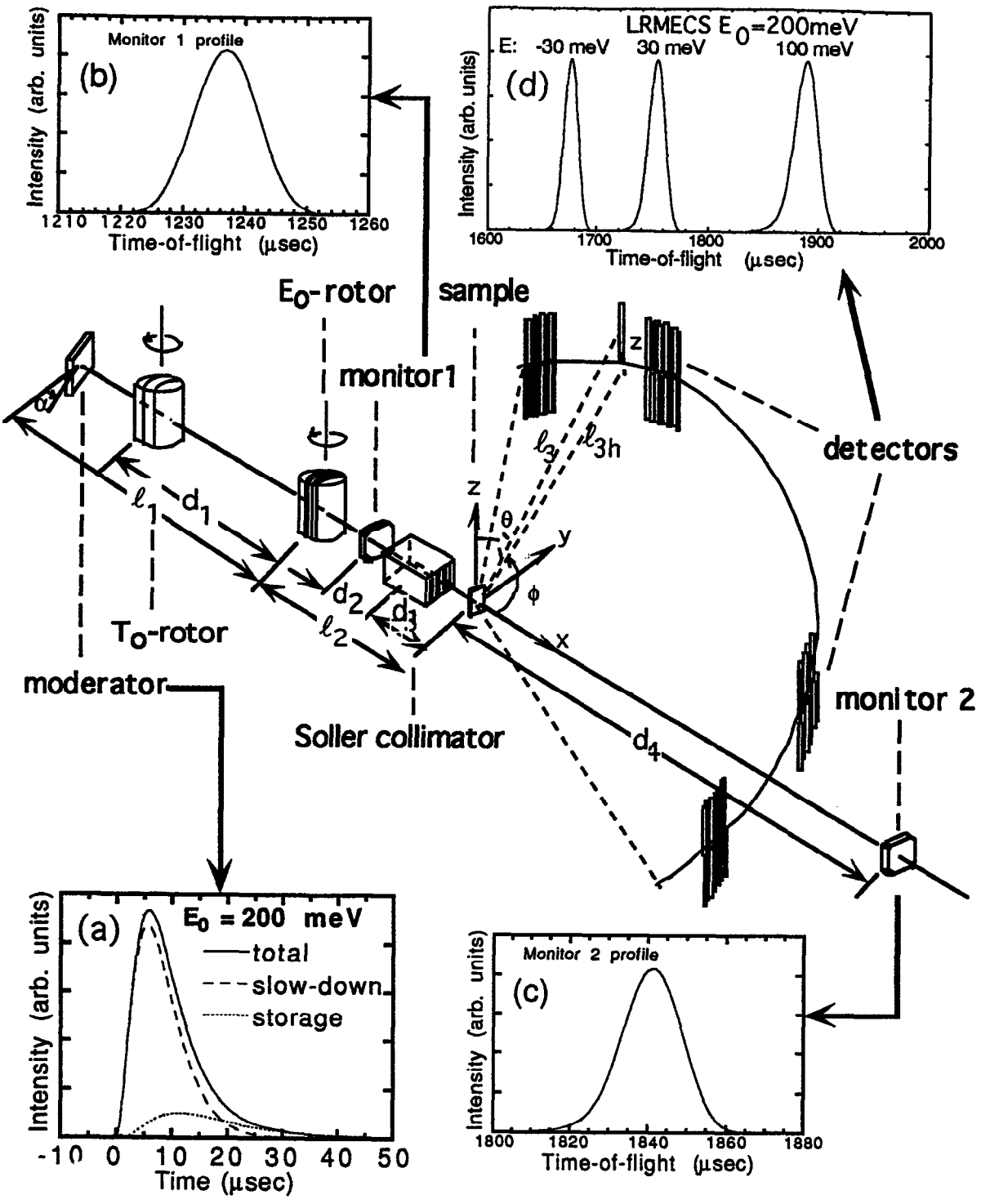

Figure 1. A schematic layout of the IPNS chopper spectrometers. The parameters for the HRMECS and LRMECS instruments are listed in Table I. Panels: (a) the source emisiion time distribution for neutron energy of 200 meV; (b-c) the calculated intensity profiles of the LRMECS monitors; and (d) the calculated resolution functions for a LRMECS detector at energy transfers -30, 30 and 100 meV.

range makes the data treatment impractical. In this paper, we present a method which overcomes these difficulties. It relies on a satisfactory parameterization of the resolution function by a simple analytic expression. In the process of data analysis the pulse-shape parameters are first obtained from a fit of the monitor spectra which are recorded as a part of the experimental data. Second, the resolution functions, calculated numerically by the convolution integral over a coarse grid of energy transfers, are fitted by an analytic expression. The process yields a set of five parameters for the resolution function at each energy. Since these parameters vary smoothly over the entire energy range of interest, their values for any specific energy transfer can be obtained from interpolation over the energy grid. Finally, the resolution functions are evaluated and applied to data analysis using the analytic formula.

Table I. Instrumental parameters for the HRMECS and LRMECS chopper spectrometers.

Parameters		HRMECS	LRMECS
α	(deg.)	-18	18
ℓ_1	(m)	12.71	7.02
ℓ_2	(m)	1.15	1.10
ℓ_{3h}	(m)[a]	4	2.5
z	(m)	0.23	0.0
d_1	(m)	5.37	1.27
d_2	(m)	0.18	0.13
d_3	(m)	0.65	0.35
d_4	(m)	5.12	3.26
ϕ	(deg.)	-20 to 20, 80 to 140	-10 to 120

[a]HRMECS detector length: 45.7 cm

LRMECS detector length: 45.7 cm for $\phi>25°$, 22.9 cm for $3°<\phi<25°$, 10.2 cm for $\phi<3°$

II. Method of calculation

1. Parametric formulation of the resolution function

Our study shows that the pulse-shape parameters mainly control the asymmetry of the resolution profile whereas other components of the spectrometers affect the overall width. Therefore, we expect that for a given mean incident energy the counting rate as a function of time t at the detector can be described quantitatively by a convolution of the pulse-shape function with a response function of the spectrometer:

$$C(t)=\frac{1}{\ell}\int_0^{\infty}dt'\int_{-\infty}^{\infty}dt''f(t')g(t'')\delta(t-\frac{\ell}{\ell_1}t_0+\frac{\ell_2+\ell_3}{\ell_1}t'-\frac{\ell}{\ell_1}t'') \qquad (1)$$

for elastic scattering, where $\ell=\ell_1+\ell_2+\ell_3$ (see Fig. 1), t_0 is the chopper opening time, $f(t)$ is the Ikeda-Carpenter function for a given energy (or neutron speed v)

$$f(t) \equiv P(v,t) = (1-R)(at)^2 \exp(-at) + \frac{Ra^2 b}{(a-b)^3}\left\{2\exp(-bt) - \left[2 + 2(a-b)t + (a+b)^2 t^2\right]\exp(-at)\right\}, \quad (2)$$

$g(x)$ is the spectrometer response function given by a Gaussian function

$$g(x) = \frac{1}{\sqrt{2\pi}\sigma}\exp\left[-\frac{1}{2}\left(\frac{x}{\sigma}\right)^2\right]. \quad (3)$$

The advantage of this expression is its simple analytic form which requires much less computer time for evaluation than the previous formalism. It can be shown that $C(t)$ can be written as

$$C(t) = \frac{A}{\ell}\frac{1}{\sqrt{2\pi}\sigma}\left\{\begin{array}{l}(1-R)a^2 C_2(a,t) \\ +\frac{Ra^2 b}{(a-b)^3}\left[2C_0(b,t) - \left((a-b)^2 C_2(a,t) + 2(a-b)C_1(a,t) + 2C_0(a,t)\right)\right]\end{array}\right\}, \quad (4)$$

where

$$C_0(x,t) = \sqrt{\frac{\pi}{2}}\left(\frac{\sigma\ell}{\ell_2+\ell_3}\right)\exp\left(v_{\min}^2 - u_{\min}^2\right) erfc(v_{\min}), \quad (5)$$

$$C_1(x,t) = \left(\frac{\sigma\ell}{\ell_2+\ell_3}\right)^2 \exp\left(v_{\min}^2 - u_{\min}^2\right)\left[\exp(-v_{\min}^2) - \sqrt{\pi}v_{\min} erfc(v_{\min})\right], \quad (6)$$

$$C_2(x,t) = \sqrt{2}\left(\frac{\sigma\ell}{\ell_2+\ell_3}\right)^3 \exp\left(v_{\min}^2 - u_{\min}^2\right)\left[\sqrt{\pi}\left(\tfrac{1}{2} + v_{\min}^2\right) erfc(v_{\min}) - v_{\min}\exp(-v_{\min}^2)\right], \quad (7)$$

and

$$v_{\min} = u_{\min} + \frac{x}{\sqrt{2}}\left(\frac{\sigma\ell}{\ell_2+\ell_3}\right), \quad (8)$$

$$u_{\min} = \frac{1}{\sqrt{2}\sigma}\left(\frac{\ell_1}{\ell}t - t_0\right), \quad (9)$$

$$erfc(z) = \frac{2}{\sqrt{\pi}}\int_{v_{\min}}^{\infty} dz \exp(-z^2). \quad (10)$$

For elastic scattering only three parameters, the normalization constant A, the Gaussian width σ and t_0 need to be determined.

2. Pulse-shape parameters

An observed beam-monitor intensity profile bears an image of the transmitted neutron pulse shape that is reversed in time due to the pin-hole-camera effect of the energy selecting rotor and broadened by the instrumental response functions. Using numerical integration methods and the measured pulse-shape functions[2], we demonstrated previously[1] the ability to accurately calculate the monitor spectra over a wide range of incident energies for the IPNS chopper spectrometers. Here we show that fitting the observed monitor spectra by $C(t)$ given in Eq. (4) can provide an estimate of the energy-dependent pulse-shape parameters, a, b, R, for the Ikeda-Carpenter function. As an example Fig. 2 shows the results of a fit of the LRMECS

monitor 2 counting rate as a function of time for a neutron energy of 200 meV. We find that the fits can be applied successfully to estimate the pulse-shape parameters for neutron energies ranging from 4 to 2000 meV for both the HRMECS and LRMECS spectrometers. Once the pulse-shape parameters are determined for an incident neutron energy, the resolution time-of-flight profiles at a few selected energy transfers are calculated by the technique of numerical integration [Eqs. (14-15) of Ref. 1]. These calculated resolution profiles are then fitted by a parametric representation of the resolution function according the following procedure.

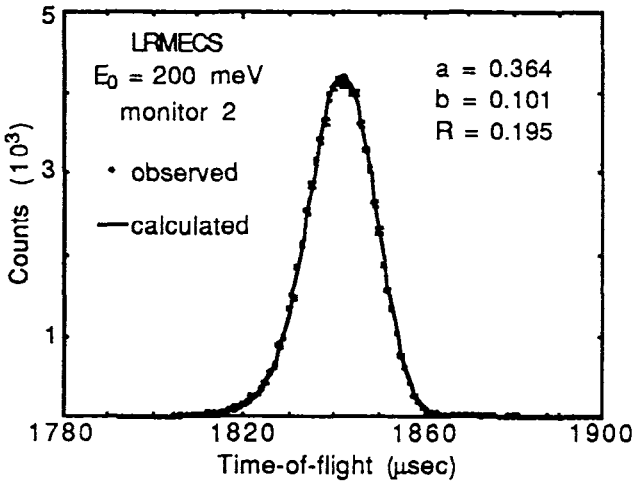

Figure 2. The monitor 2 spectrum of LRMECS with an incident neutron energy of 200 meV. The pulse-shape parameters, a, b, and R were determined by a least-squares fit.

3. Calculation of the resolution function $R(E'-E)$

For inelastic scattering, we find that Eq. (1) can still describe accurately the resolution function provided that the arrival time at the detector, t_d, for a neutron of final speed v_f is re-scaled to the elastic position, i. e.,

$$t \equiv t_d - \frac{\ell_3}{v_f} + \frac{\ell_3}{v_i}, \tag{11}$$

where v_i is the neutron initial speed. In this case, in addition to A, t_0 and σ, a, b and R are also treated as adjustable parameters, which we denote as a^*, b^* and R^*. They no longer carry any physical meaning as pulse-shape parameters.

Fig. 3. shows several examples of fitting the LRMECS resolution time-of-flight profiles calculated by numerical integration of the analytic expression Eq. (4). As it can be seen, the resolution profiles are adequately described by the parametric expression. The changes in the asymmetry of the profiles with energy transfer are accommodated by the varying proportions of the slowing-down and storage terms in the pulse-shape function as a^*, b^* and R^* change whereas the widths are effected by varying σ. Several sets of a^*, b^*, R^*, σ and t_0 are first obtained this way over a coarse grid of energy transfer. Since these parameters are slowly varying variables with respect to the energy transfer, their values at any energy transfer can be

found by interpolation. The resolution functions, $R(E'-E)$, at an energy transfer E can then be calculated using Eq. (4) and the relation:

$$t=\frac{\ell}{v_i}-\frac{\ell_3}{v_f}+\frac{\ell_3}{\sqrt{v_f^2-\frac{2E'}{m}}}, \tag{12}$$

where m is the neutron mass. It is this computer-time saving calculation that makes the application practical for the analysis of large volume data sets. The parameters t_0, σ, a^*, b^*, R^* and the energy transfer E, and the results of interpolation in the -30 < E < 130 meV region are shown in Fig. 4 for LRMECS with an incident energy of 200 meV. Examples of the calculated resolution functions $R(E'-E)$ at five E values are shown in Fig. 5.

III. Results and Discussion

We have tested the application of the resolution calculations by the aforementioned method for the analyses of a variety of chopper spectrometer data[3]. The results are satisfactory. Several computer codes were written for this purpose. A typical procedure for the use of this resolution calculation is outlined in Fig. 6. We anticipate that this method can be used for data interpretation so as to simulate a predicted spectrum when a theoretical model is available, or to extract intrinsic parameters from an observed spectrum in conjunction with a least-squares or maximum-entropy analysis. This method has been applied for analysis of chopper spectrometer data, such as crystal-field studies[4] of rare-earth materials. We find that the resolution calculation is useful in providing a quantitative comparison of the theory with experiment and a measure of the intrinsic crystal-field linewidths.

In summary, we describe a parametric formulation and an algorithm which afford an efficient calculations of the resolution function for a pulsed-source chopper spectrometer.

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References:

1. C.-K. Loong, S. Ikeda and J. M. Carpenter, Nucl. Instr. and Meth. **A260**, 381 (1987).
2. S. Ikeda and J. M. Carpenter, Nucl. Instr. and Meth. **A239**, 536 (1985).
3. C.-K. Loong, L. I. Donley, G. E. Ostrowski, R. Kleb, J. P. Hammonds, L. Soderholm, and S. Takahashi, this Proceedings.
4. See for example, C.-K. Loong, L. Soderholm, J. P. Hammonds, M. M. Abraham, L. A. Boatner, and N. M. Edelstein, J. Phys.: Condens. Matter. (in press)

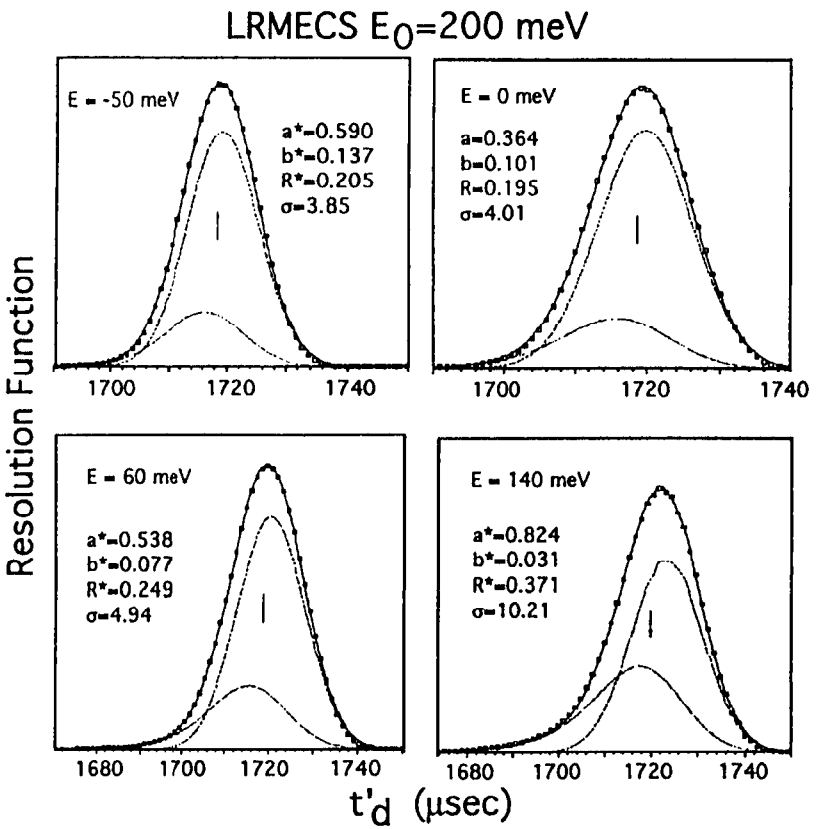

Figure 3. The least-squares fits of the calculated resolution functions for LRMECS with an incident energy of 200 meV by the analytic expression of Eq. (4). The dashed and dotted curves correspond to the two components of the pulse-shape function of Eq. (2).

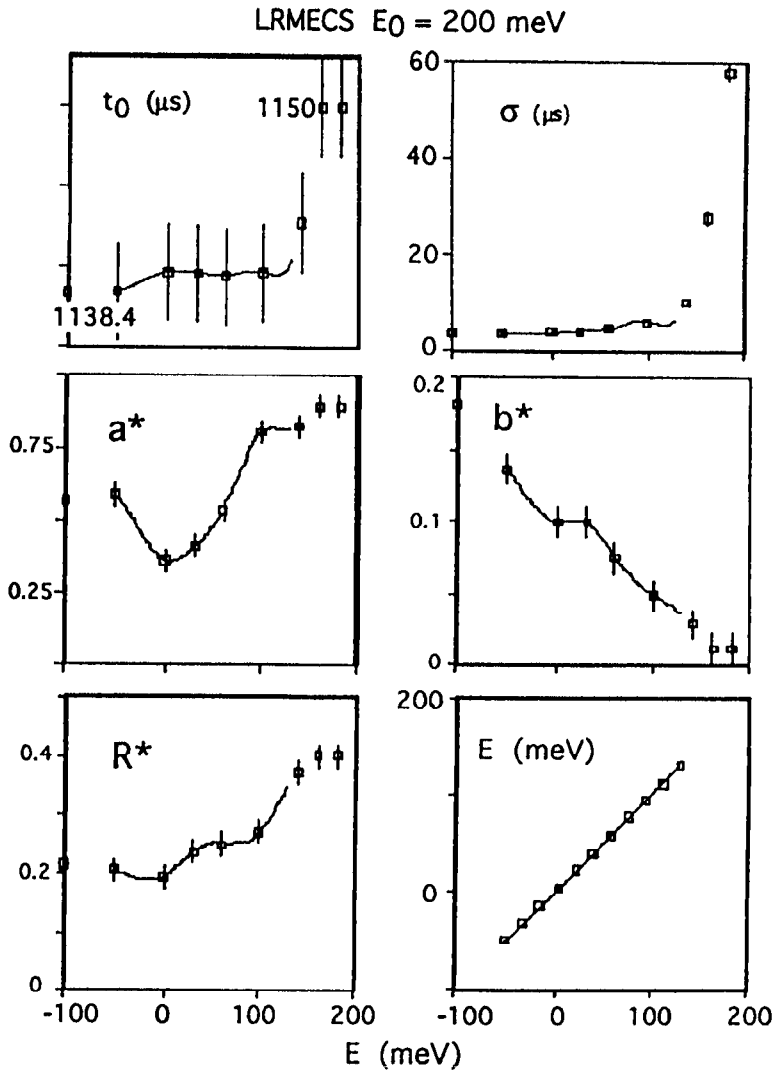

Figure 4. Variations of the parameters t_0, σ, a*, b*, R* and the calculated energy transfer E over the -100 to 160 meV energy region for LRMECS with E_0 = 200 meV. The curves represent the results of interpolation over the energy range of -30 to 130 meV.

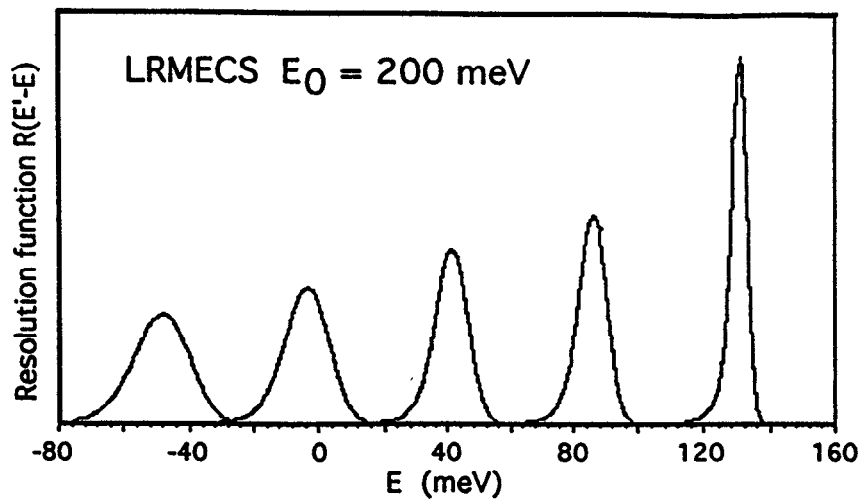

Figure 5. Calculated resolution functions R(E'-E) at five energy transfers for LRMECS with an incident energy of 200 meV.

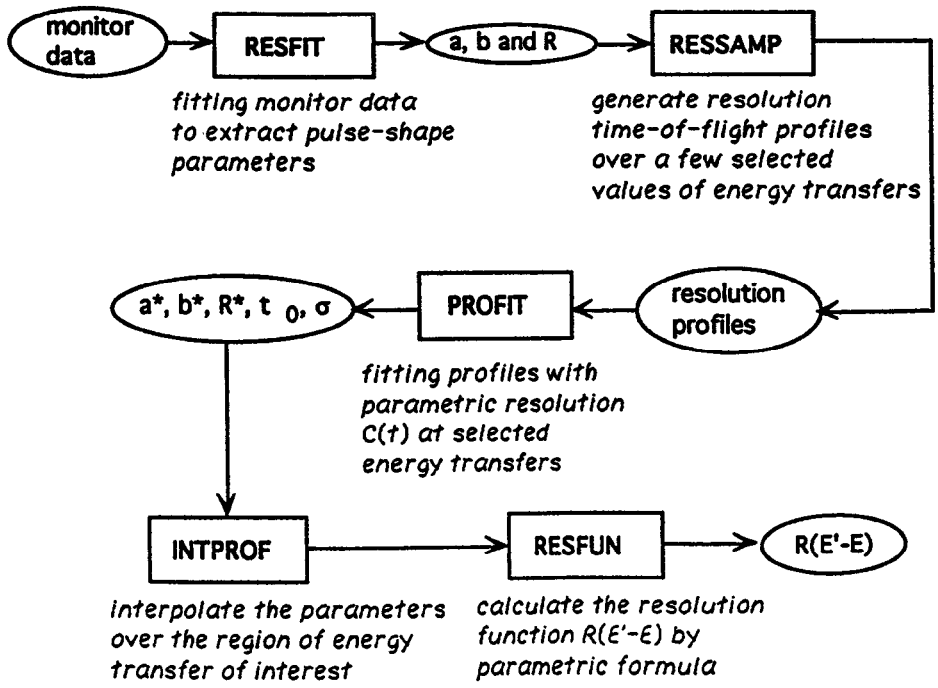

Figure 6. A flow chart for a typical resolution calculation in a data analysis.