AIP | Review of Scientific Instruments

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A. A. Istratov

Citation: Review of Scientific Instruments **68**, 3861 (1997); doi: 10.1063/1.1148038
View online: http://dx.doi.org/10.1063/1.1148038
View Table of Contents: http://scitation.aip.org/content/aip/journal/rsi/68/10?ver=pdfcov
Published by the AIP Publishing

The resolution limit of traditional correlation functions for deep level transient spectroscopy

A. A. Istratov[a)]
Department of Materials Science and Mineral Engineering, University of California at Berkeley, Berkeley, California 94720-1760

(Received 24 June 1997; accepted for publication 7 July 1997)

The factors limiting the resolution of the traditional correlation deep level transient spectroscopy (DLTS) are revealed and analyzed. It is shown that all weighting functions proposed to date provided nonsymmetrical rate windows, effectively filtering out slow transients, but were mediocre filters for fast transients. It is argued that it was the response to fast transients which actually limited the resolution of the correlation DLTS. The resolution limit of previously published weighting functions is determined. It is shown that the limitations are inherent in the earlier approach to the devising of weighting functions rather than in the correlation procedure itself. It can be overcome using new weighting functions based on the Gaver-Stehfest algorithm for the inverse Laplace transformation. © *1997 American Institute of Physics.* [S0034-6748(97)01810-8]

I. INTRODUCTION

Deep level transient spectroscopy (DLTS)[1] has become an important tool for the investigation of deep levels in semiconductors. The sensitivity of a DLTS setup, i.e., the ability to detect weak exponential decays, and its selectivity, is strongly affected by the choice of the DLTS correlation function. More than 20 different correlation functions have been proposed during the past 20 years[2–11] (Fig. 1). According to the theory of signal processing, the highest sensitivity is provided by the weighting function, which has the form of the noise-free signal itself, and therefore for a DLTS system it should be a decaying exponential.[2] Unfortunately, compared to other known weighting functions, the exponential correlator had the broadest DLTS peaks, i.e., the worst selectivity. A lot of research effort has been spent on searching for a correlation function with a sensitivity, comparable to that of the exponential correlator, but giving much better resolution. Nevertheless, until now it was not clear whether there is a limit to the resolution capacity of correlation DLTS and, if it exists, what is the cause of this limitation.

In the first part of the article, analytical approximations for the low-temperature and high-temperature sides of a DLTS peak are obtained. It is shown that a filter with arbitrary high steepness of the low-temperature side of the DLTS peak can be constructed. On the other hand, almost all reported to-date weighting functions have had the same form of the high-temperature side, which actually limited the resolution. The resolution limit of previously published weighting functions is determined.

In the second part of the article it is shown that this resolution limit is a shortage of reported weighting functions rather than a general limitation of correlation DLTS. Two new weighting functions, based on the Gaver-Stehfest algorithm, are discussed. As these weighting functions are actually narrow-band filters, i.e., effective filters both for fast and slow transients, they do not have the resolution limitations of traditional functions.

[a)]On leave of absence from the Institute of Physics of St. Petersburg State University, Ulianovskaya 1, Petrodvoretz, St. Petersburg, 198904 Russia; Electronic mail: istratov@socrates.berkeley.edu

II. ASYMPTOTIC ANALYSIS OF THE LOW-TEMPERATURE SIDE OF THE DLTS PEAK

The output signal of a DLTS correlator is generally given by

$$S(\tau_s)=t_c^{-1}\int_{t_d}^{t_d+t_c}\exp(-t/\tau_s)W(t-t_d)dt, \tag{1}$$

where W is the weighting function, S is the output DLTS signal, t_c is the duration of the correlation, and t_d is the delay time between the end of the filling pulse and the beginning of the correlation. The delay time is usually introduced to improve selectivity or to avoid distortions of the signal due to overload of the capacitance meter just after the filling pulse.

Let us consider the output signal of the DLTS correlator if the input capacitance transient has the time constant $\tau_s \gg \tau_0$, $\tau_0 \sim (0.1–0.6)t_c$ being the emission rate at which the DLTS signal is a maximum. For $t<[0,t_c+t_d]$ the ratio t/τ_s will be much less than unity and the exponent under the integral in Eq. (1) can be expanded in a Taylor's series:

$$S(\tau_s)=t_c^{-1}\int_{t_d}^{t_d+t_c}\left(1-\frac{t}{\tau_s}+\frac{1}{2}\frac{t^2}{\tau_s^2}-\cdots\right)W(t-t_d)dt. \tag{2}$$

If the weighting function satisfies the condition

$$\int_{t_d}^{t_d+t_c}t^k\cdot W(t-t_d)dt=0, \quad 0\leqslant k<k_0 \tag{3}$$

then the first k_0 terms in Eq. (2) can be neglected and Eq. (1) can be approximated by

$$S(\tau_s)\approx t_c^{-1}\int_{t_d}^{t_d+t_c}\text{const}\cdot\frac{t^{k0}}{\tau_s^{k0}}\cdot W(t-t_d)dt=\text{const}\cdot\tau_s^{-k0}. \tag{4}$$

The output signal of the correlator will be proportional to τ_s^{-k0} for slow transients. A filter with the characteristic $S(\tau_s)\sim\tau_s^{-k0}$ is called in electronics ''the k_0-order filter,''

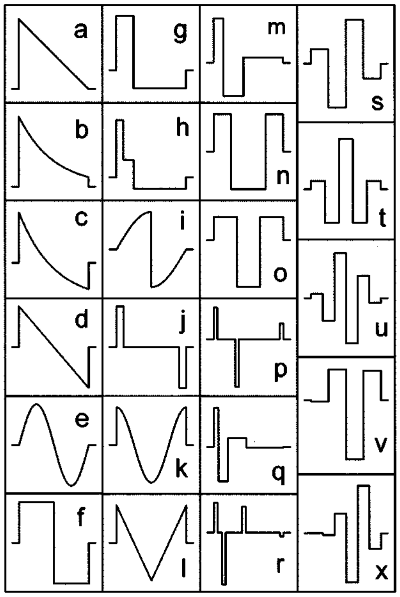

FIG. 1. Waveforms of different weighting functions: (a) linear ramp, $w = 1 - t^*$, t^* being the normalized time $t^* = (t - t_d)/t_c$, $t^* \subset [0,1]$; (b) exponential correlator, $w = \exp(-2t^*)$; (c) shifted exponential, $w = \exp(-2t^*) + [\exp(-2) - 1]/2$; (d) shifted linear ramp, $w = 1/2 - t^*$; (e) sine wave, $w = \sin(2\pi t^*)$; (f) rectangular lock-in, $w = \mathrm{sign}(1/2 - t^*)$, $\mathrm{sign}(x)$ is defined as -1, if $x < 0$, and 1, if $x \geqslant 0$; (g) rectangle function of Crowell, steps height 1, $-1/3$, steps durations $0.25t^*$, $0.75t^*$; (h) rectangle function of Hodgart, steps height 1, 0.309, -0.196, steps duration $0.1t^*$, $0.15t^*$, $0.75t^*$; (i) split sine wave, $w = \sin(\pi t^*)\mathrm{sign}(1/2 - t^*)$; (j) double boxcar, $w = 1$, $0 \leqslant t^* < 0.1$, $w = 0$, $0.1 \leqslant t^* \leqslant 0.9$, $w = -1$, $0.9 < t^* \leqslant 1$; (k) cosine, $w = \cos(2\pi t)$; (l) triangular, $w = 1 - 4t^*$, $0 \leqslant t^* < 0.5$, $4t^* - 3$, $0.5 \leqslant t^* < 1$; (m) three-steps function of Crowell, steps height 1, $-3/4$, 1/8, steps duration 1/7, 2/7, 4/7; (n) square wave, steps height 1, -1, 1, steps duration 1/4, 1/2, 1/4; (o) HiRes-3, height of equal-duration steps -1, 2, -1; (p) three-point function of Dmowski, $w = 1$, $-3/2$, 1/2 at $t^* = 0$, 1/3, 1, strobes width 0.05; (q) four-steps function of Crowell, steps height 1, $-7/8$, 7/32, $-1/64$, steps duration 1/15, 2/15, 4/15, 8/15; (r) four-point function of Dmowski, strobs height 1, $-7/4$, 7/8, $-1/8$, strobs positions 0, $t^*/7$, $3t^*/7$, t^*, width of strobs $\Delta t^* = 0.05$; (s) HiRes-4, height of equal-width steps is 1, -3, 3, -1; (t) HiRes-5, height of equal-width steps is 1, -4, 6, -4, 1; (u) HiRes-6, height of equal-width steps is -1, 5, -10, 10, -5, 1; (v) GS-4, height of equal-width steps is -1, 25, -48, 24; (x) GS-6, height of equal-width steps is 1, -97, 1002, -2526, 2430, -810.

and following Crowell *et al.*,[3] we use the same term to denote correlators with this kind of characteristic. Filters from the first to the fifth and higher orders are known and were proposed as weighting functions. Crowell *et al.*,[3] Thurzo *et al.*,[4] and Hodgart[5] developed techniques for constructing steplike weighting functions of a given order. Therefore, the low-temperature side of the DLTS peak can be made as steep as required and does not limit the resolution of correlation DLTS.

III. ANALYSIS OF THE HIGH-TEMPERATURE SIDE OF THE DLTS PEAK AND THE INFLUENCE OF THE DELAY TIME ON PARAMETERS OF THE CORRELATORS

The dependence $S(\tau)$ for $\tau \ll \tau_0$ (high-temperature side of the DLTS peak) is determined by fast transients, decaying quickly after the filling pulse. As the area under the plot of a decaying exponent $\exp(-t/\tau)$ is proportional to τ, an arbitrary weighting function [even $W(t) \equiv \mathrm{const}$] will provide at least a first-order filter for the fast transients:

$$S(\tau_s) = \int_0^{t_c} \exp(-t/\tau_s)\, dt = \tau_s \cdot \mathrm{const} \to 0, \quad \tau_s \to 0. \tag{5}$$

The waveform of the weighting function W can in principle increase the order of the filter for fast transients. In fact, our simulations revealed that almost all previously reported weighting functions are only first-order filters for fast transients, independently of the order of the filter for slow transients. Only two exceptions were found—sine wave and split sine wave [Figs. 1(e) and 1(i)] which are the second-order filters for fast decays [$S(\tau) \sim \tau^2$ for $\tau \to 0$]. According to our analysis, the waveform of the correlation function slightly affected the dependence $S(\tau_s) \sim \tau_s$ or $S(\tau_s) \sim \tau_s^2$, shifting it along the τ/τ_0 axis, or changing its slope within about 5%.

The most efficient DLTS peak form, from the point of view of selectivity, would be the symmetric form. For the filter of the order k it should be $S(\tau) \sim \tau^{-k}$ for $\tau \gg \tau_0$ and $S(\tau) \sim \tau^k$ for $\tau \ll \tau_0$. Consequently, the best way to increase the resolution of the existing weighting functions would be to improve its fast-transient response. It can partly be done, introducing a delay time t_d between the end of the filling pulse and the beginning of the weighting function. The idea of increasing the resolution of the spectrum by delaying the weighting function briefly mentioned in the early works of Miller.[2] Crowell *et al.*,[3] Tokuda *et al.*[6,7] and later Dmowski *et al.*[8] obtained analytical expressions for the determination of rate windows of lock-in with different delay times. To obtain a straight line on the Arrhenius plot after the introduction of a delay time, it was proposed[6–10] to keep the t_d/t_c ratio fixed. This keeps the proportionality between the time constant τ_0 of the capacitance relaxation at the point of maximum of the DLTS peak, and the duration of the weighting function t_c. Nolte and Haller[11] demonstrated that the correlation of the exponential transient is equivalent to the Laplace transform of the weighting function and showed that the functional form of the high-temperature (relative to the position of the DLTS peak) response is simply the Laplace transform of the leading term in the Taylor's expansion of the weighting function. To decrease the width of the DLTS peak, the leading term in the Taylor's expansion of the weighting function should be of as high an order as possible, which is nothing else than weighting to later times.[11]

What actually happens to the form of the DLTS peak with increasing delay time can be seen in Fig. 2. Curve 1 is the dependence of the output signal of a typical DLTS correlator (double boxcar) on the time constant of the input exponential decay without delay time. The slopes of both low-temperature ($\tau \gg 1$) and high-temperature ($\tau \ll 1$) sides of the dependence in logarithmic scale are unity, which corresponds to the first-order filters both for slow and fast transients. The introduction of the delay time t_d changes the dependence Eq. (5) to the form

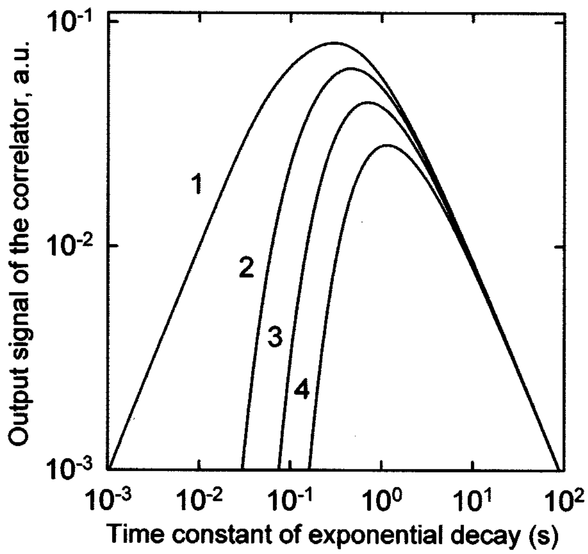

FIG. 2. Dependence of the output signal of the typical weighting function (double-boxcar correlator) on time constant of exponential decay for different values of delay time: curve 1: $t_d=0$, curve 2: $t_d=0.1t_c$; curve 3: $t_d=0.3t_c$, curve 4: $t_d=0.7t_c$.

$$S(\tau_s)=\int_{t_d}^{t_d+t_c}\exp(-t/\tau_s)dt=\text{const}\cdot\exp(-t_d/\tau_s)\cdot\tau_s,\quad \tau_s\to 0. \tag{6}$$

The exponential $\exp(-t_d/\tau_s)$ is a fast decaying function for $\tau_s\to 0$, and it suppresses, for small values of τ_s, any linear or quadratic dependence of $S(\tau_s)$. The fast-transient side of the dependence $S(\tau_s)$ becomes nonlinear in logarithmic scale (curves 2–4, Fig. 2). Its slope (which was unity before the introduction of the delay time) ranges between 2 and 3 in the part of the dependence which is the most important for practical purposes, close to the DLTS maximum $[1>S(\tau_s)/S(\tau_0)>0.1]$.

Another consequence of Fig. 2 and Eq. (6) is that a relatively small delay time is required to make the slope of the fast-transient side of the dependence be dominated by the exponential $\exp(-t_d/\tau_s)$. Obviously, curves 2, 3, and 4 in Fig. 2, corresponding to delay times $0.1t_c$, $0.3t_c$, and $0.7t_c$, respectively, have approximately the same slope of the fast-transient side. The delay time, beyond a certain value, does not significantly change the form of the peak, but reducing the amplitude of the DLTS peak increases the signal-to-noise ratio.

The influence of the delay time on the parameters of several correlation functions was discussed previously.[9] The optimum value of the delay time, which provided a noticeable increase of the resolution (up to 20%) almost without losses in the signal-to-noise ratio was individual for each weighting function and lied in $t_d\sim(0.02 \text{ to } 0.07)t_c$ range.

The optimum values of delay time for the weighting functions, presented in Fig. 1, and their parameters with optimum delay times are given in Table I. The width w of the DLTS peak was calculated as a ratio between the time constants of exponential relaxations $\tau_{\min}$ and $\tau_{\max}$ at which half of the maximum amplitude of the DLTS peak is reached:

TABLE I. Parameters of the weighting functions from Fig. 1, calculated with the optimum delay time.

Order of the filter	Weighting function	Optimum delay time (t_d/t_c)	DLTS peak width (w)	Signal-to-noise ratio (SNR)
0(1)	linear ramp	0.076	15.5	0.33
	exponential	0.086	15.6	0.32
1	shifted exponential	0.082	16.2	0.21
	shifted linear ramp	0.077	15.9	0.20
	sine	0	15.2	0.18
	lock-in	0.048	15.7	0.18
	rectangular (Crowell)	0.057	16.5	0.19
	rectangular (Hodgart)	0.075	16.8	0.18
	split sine	0	14.2	0.13
	double boxcar	0.131	16.5	0.13
2	cosine	0.032	8.8	0.093
	triangular	0.037	8.8	0.092
	three steps (Crowell)	0.018	9.4	0.091
	square wave	0.023	8.8	0.084
	HiRes-3	0.019	8.5	0.069
	three point (Dmowski)	0.040	9.7	0.065
3	four-steps (Crowell)	0.008	8.0	0.053
	four point (Dmowski)	0.011	7.9	0.047
	HiRes-4	0.011	6.7	0.029
4	HiRes-5	0.007	5.9	0.013
5	HiRes-6	0.005	5.4	0.0058
GS	GS-4	0	5.26	0.0159
	GS-6	0	3.42	0.00111

$$w=\tau_{\max}/\tau_{\min}. \tag{7}$$

The signal-to-noise ratio SNR of the output signal was determined as a ratio of the output signal S, calculated from Eq. (1), provided the amplitude of the input capacitance transient was unity, and noise N: SNR=S/N. Noise N was found from the expression[3,12]

$$N=\left(\int_{t_d}^{t_d+t_c}[W(t-t_d)]^2dt\right)^{1/2}. \tag{8}$$

The inverse value SNR^{-1} gives an estimate of the signal-to-noise ratio, of the input transient which is required to obtain a signal-to-noise ratio exceeding unity in the output spectrum. It should be noted that the SNR value (Table I) is calculated for a single transient. Averaging the sequence of transients noticeably improves the signal-to-noise ratio of the DLTS spectrum.

IV. THE RESOLUTION LIMIT OF TRADITIONAL CORRELATION DLTS

As indicated in Table I, going to the next filter order leads to at least a twofold decrease in the signal-to-noise ratio. However, the improvement of the peak width is much less significant, especially for the high-order filters. If we plot the signal-to-noise ratio of different correlators versus their peak width, we will see that this dependence decreases linearly with the decreasing peak width (Fig. 3) and crosses the horizontal axis at $w\approx 4.4$. This value gives the resolution

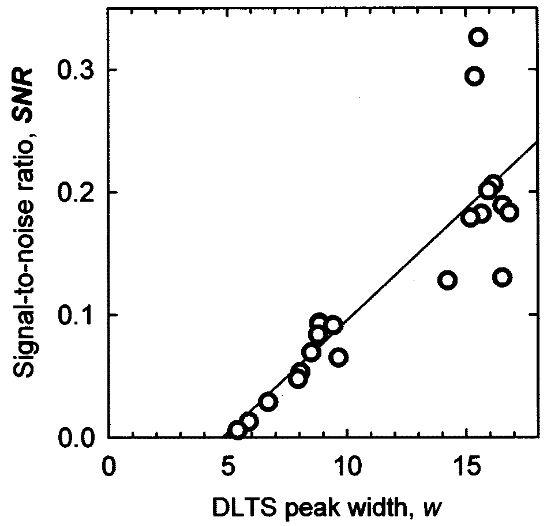

FIG. 3. Dependence of the signal-to-noise ratio SNR of DLTS spectra, obtained with different correlation functions with the optimum delay time on the width of DLTS peak (data from Table I with the exception of functions GS-4 and GS-6, discussed in Sec. V).

limit of traditional correlation functions with the optimized delay time. The existence of such a limit has a simple explanation.

High resolution DLTS requires, using Lang's terminology, very narrow rate windows with steep sides, so that only transients with the time constants close to the middle of the rate window would give a nonzero signal. When the filter order is increased, the low-temperature side of the peak becomes steeper, improving the filtering of slow transients. At the same time, the response for the fast transients remains the same. Therefore, the rate windows provided by the traditional correlation functions are generally not symmetric, and become less symmetric with increasing order of the filter. The high-temperature side of the peak does not depend on the filter order and provides the limitation for the resolution capacity.

The most efficient peak form, from the point of view of resolution capacity, is the symmetric form, which is the case, as the calculations show, for the second- and third-order filters. The improvement in resolution of the weighting functions of higher order is not significant compared to the losses in the signal-to-noise ratio, and their usage is therefore not justified. The resolution, which can be obtained with the third-order weighting function, is about $w \approx 6$ (see Table I), which corresponds to the energy resolution $\Delta E/E$ of about 8.5%. This value is indeed much worse than the values $w < 2$, which can be obtained by the methods of inverse Laplace transform.[13]

The value of the resolution limit of previously published weighting functions can also be obtained from the following considerations: the linewidth of the lock-in correlator without delay time ($t_d = 0$), which has a symmetrical characteristic, is $w = 18.3$ (note that all parameters in Table I are given for $t_d = t_{d\,\mathrm{opt}}$). Assuming that increasing the order of the filter, we make the slope of the slow-transient side arbitrary steep, keeping the fast-transient side unchanged, the linewidth decreases to the half of the initial width on the logarithmical scale, i.e., to the value $(18.3)^{1/2} \approx 4.3$, which is very close to the estimate $w \approx 4.4$.

V. A NEW CLASS OF NARROW-BAND SYMMETRICAL FILTERS: WEIGHTING FUNCTIONS, BASED ON GAVER–STEHFEST ALGORITHM

A better way to improve the resolution is to find a correlation function which would be an effective filter for both slow and fast transients. The weighting functions satisfying these requirements can be obtained from the formula derived by Stehfest[14] from the statistical expectation function defined by Gaver.[15] The Gaver–Stehfest algorithm is usually considered a method of numerical inversion of the Laplace transform. Given a Laplace image [in our case an experimental decay curve $f(t)$], the algorithm calculates an approximation for the inverse $g(\lambda)$:

$$g(\lambda) = \frac{\ln(2)}{\lambda} \sum_{m=1}^{N} K_m \cdot f\left(\frac{m \ln(2)}{\lambda}\right), \tag{9}$$

where

$$K_m = (-1)^{m+(N/2)} \sum_{k=(m+1)/2}^{\min(m,N/2)} \times \frac{(2k)!\,k^{1+(N/2)}}{(N/2-k)!\,k!\,(k-1)!\,(m-k)!\,(2k-m)!}. \tag{10}$$

Theoretically $g(\lambda)$ becomes more accurate, the greater the value of N. Practically, however, rounding errors deteriorate the results if N becomes too large.

The Gaver–Stehfest algorithm calculates the inverse Laplace transformation as a linear combination of values of capacitance of the sample at subsequent instants of time t_m. For each value of λ an individual set of t_m is used. Thus for a given transient $f(t,T)$ the whole dependence $g(\lambda)$ can be restored.

Of course, Eq. (9) can be restricted to only one emission rate λ and the temperature of the sample varied until the emission rate passes into the rate window λ. In this case, to calculate the inverse transform Eq. (9) at one point, the values of capacitance at equidistant points $t_1, t_2, .. t_N$ and the set of coefficients K_m are required. The Gaver–Stehfest algorithm will be reduced to a weighting function, consisting of N strobes at $t = t_m$, $m = 1,..,N$, with the amplitudes K_m [Eqs. (9) and (10)]. The waveforms of the simplest functions for $N = 4,6$ [N should be even in Eq. (9)] are presented in Fig. 1 (v,x), the parameters of the functions—in Table I.

The detailed discussion of the properties of these new weighting functions is beyond the scope of this paper and will be published separately.[16] The most important feature of the new weighting functions is that they provide narrow-band filters with rather symmetrical characteristics. Even the simplest four-step filter GS-4 has better resolution than the more complicated filter of the fourth order HiRes-5. Filter GS-6 yields a resolution as high as $w \sim 3.4$. This value is higher than the resolution limit ($w \approx 4.4$) of traditional correlation DLTS, estimated above. However, this function can be employed only if the signal-to-noise ratio in the capacitance transient is high enough. A good estimate for the required signal-to-noise ratio is given by the value $\mathrm{SNR}^{-1} \approx 900$. If the noise-limited sensitivity of the capacitance meter is about $\Delta C/C \approx 10^{-4}-10^{-5}$, which is a typical value, then the function GS-6 may be used to study defects with concentrations about $N_T/N_D = 2\Delta C/C \sim 0.2-0.02$ even without averaging the transients.

ACKNOWLEDGMENTS

The author gratefully acknowledges continuing discussions on capacitance spectroscopy with O. F. Vyvenko, which stimulated the appearance of this paper. Overall support and interest in this work by E. R. Weber, critical remarks on the manuscript made by E. Edelson and V. M. Ustinov are acknowledged. This work was partly supported by NREL Subcontract XD-2-11004-3.

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