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Citation: Journal of Applied Physics **82**, 2965 (1997); doi: 10.1063/1.366269
View online: http://dx.doi.org/10.1063/1.366269
View Table of Contents: http://scitation.aip.org/content/aip/journal/jap/82/6?ver=pdfcov
Published by the AIP Publishing

New correlation procedure for the improvement of resolution of deep level transient spectroscopy of semiconductors

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(Received 4 April 1997; accepted for publication 5 June 1997)

The selectivity and sensitivity of deep level transient spectroscopy (DLTS) depend significantly on the choice of the correlation function. In this article, the factors limiting the resolution of correlation DLTS are discussed. It is argued that the weighting functions reported to date provide asymmetrical rate windows, being effective filters only for slow transients. To overcome this limit, a correlation procedure, based on the Gaver–Stehfest algorithm for the inverse Laplace transformation, is proposed. Using this procedure one can obtain a temperature scanned DLTS mode resolution comparable to the resolution of sophisticated methods of inversion of the Laplace integral equation. © *1997 American Institute of Physics.* [S0021-8979(97)00518-5]

I. INTRODUCTION

Deep level transient spectroscopy (DLTS)[1] has become an important tool for the investigation of deep levels in semiconductors. The sensitivity of the DLTS system, i.e., the ability to detect weak exponential decays, and its selectivity, which permits one to distinguish two closely spaced deep levels, are strongly affected by the choice of the correlator. In the most general form, the correlation procedure is given by

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

where f is the capacitance transient, W is the weighting function, S is the output DLTS signal, t_c is the duration of the correlation, 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.

According to the theory of signal processing, the best 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 has the broadest DLTS peaks and the worst selectivity. A lot of research effort has been spent on searching for a correlation function which would have the highest possible resolution, retaining an acceptable sensitivity.[3–8] However, none of the suggested weighting functions could provide the resolution, comparable with that of sophisticated numerical methods, used for inversion of the Laplace integral equation.

Recently, the author made an extensive analysis of previously published weighting functions and established the factors, which limited the resolution of the correlation DLTS. The details of this analysis are beyond the scope of the present article and will be published elsewhere.[9] The main conclusion was that all weighting functions proposed to date provided nonsymmetrical rate windows, effectively filtering out slow transients, but being mediocre filters for fast transients. High resolution DLTS requires, using Lang's terminology, very narrow rate windows with steep sides, so that only transients with time constants close to the middle of the rate window would give a nonzero signal. Response of a correlator to slow transients with the time constant τ_s much larger than the giving DLTS maximum time constant τ_0 can be easily approximated, expanding the exponential term $f(T,t)$ under the integral in Eq. (1) 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

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

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

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

The output signal of the correlator will be proportional to $\tau_s{}^{-k0}$ for slow transients. A filter with the characteristic $S(\tau_s)\sim\tau_s{}^{-k0}$ is called in electronics "the k_0-order filter," 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 (see Ref. 9 for the review). Crowell *et al.*,[3] Thurzo *et al.*,[4] and Hodgart[5] developed a simple technique for constructing the steplike weighting functions of a given order.

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 $\tau\ll\tau_0$. In fact, our simulations revealed that

[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@snoopy.niif.spb.su or istratov@socrates.berkeley.edu 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, which are the second-order filters for fast decays $[S(\tau)\sim\tau^2$ for $\tau\rightarrow 0]$. 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 fast transients remains the same. Therefore the rate windows provided by traditional correlators are generally unsymmetrical high-pass filters: they filter out only slow transients, 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 improvement in resolution of the weighting functions of an order higher than 2–3 is not significant compared to the losses in signal-to-noise ratio, and their usage is therefore not justified.

A weighting function of the third order can in principle resolve two transients with the ratio of time constants of $w=\tau_1/\tau_2\approx 8$, which corresponds to the energy resolution ΔE/E of about 8.5%. This value can be considered as the practical resolution limit for all weighting functions proposed to date. Fortunately, it can be substantially improved by using a new class of weighting functions with symmetrical characteristics, based on the Gaver–Stehfest algorithm.

II. 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[10] from the statistical expectation function defined by Gaver.[11] The Gaver–Stehfest algorithm is usually considered a method of numerical inversion of the Laplace transform. Davies,[12] who compared 14 different methods for numerical inversion of the Laplace transform, came to the conclusion that the Gaver–Stehfest method is more accurate than most methods, which do not require calculations on the complex plane, and is the fastest among them. Given a Laplace image [in our case an experimental decay curve $f(t)$], the algorithm calculates an approximation for the inverse $g(\lambda)$:

$$g(\lambda)=\frac{\ln 2}{\lambda}\sum_{m=1}^{N} K_m\, f\left(\frac{m\ln 2}{\lambda}\right), \tag{5}$$

where

$$K_m=(-1)^{m+(N/2)} \times \sum_{k=(m+1)/2}^{\min(m,N/2)} \frac{(2k)!\,k^{1+(N/2)}}{(N/2-k)!\,k!\,(k-1)!\,(m-k)!\,(2k-m)!}. \tag{6}$$

Theoretically $g(\lambda)$ becomes the more accurate the greater the value of N. Practically, however, rounding errors deteriorate the results if N becomes too large. The optimum N is approximately equal to the number of digits the computer is working with.[8,10] This algorithm was tested by Nolte and Haller[8] with double-precision arithmetic and $N=24$. It was shown that, without noise, one can typically resolve two exponents with the ratio of time constants equal to 1.5, which corresponds to the energy resolution of 2%. This value was compared to the typical resolution of standard DLTS correlation functions between 9% and 15%, and a substantial improvement in deep level energy resolution using the Gaver–Stehfest algorithm was indicated.[8] (Note however, that 24 digits is much higher than the accuracy of a conventional analog-to-digital converter.) For a noise variance of 0.3% of the peak signal added to each data point, energy resolution is reduced to about 4%,[14] which is still much better than the best possible resolution of the conventional DLTS filter.

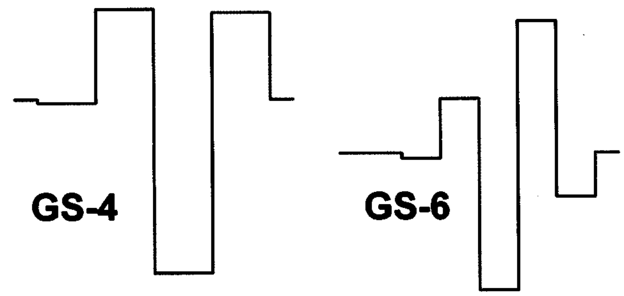

FIG. 1. Wave forms of weighting functions, based on Gaver–Stehfest algorithm. Function GS-4 consists of four steps of equal duration with the amplitudes −1, 25, −48, 24. Function GS-6 consists of six steps of equal duration with the amplitudes 1, −97, 1002, 2526, 2430, −810. The signal at the output of the correlator at the point of DLTS maximum is 0.470 for GS-4 and 1.698 for GS-6 (assuming the unity amplitude of the input exponential transients). Ratio of the time constant of the exponential transient, giving the DLTS maximum, to the duration of the weighting function, is 0.293 for GS-4 and 0.215 for GS-6. Optimum delay time t_d is zero for both functions (see Ref. 9 for more details).

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. In such a way, for a given transient $f(t,T)$, the whole dependence $g(\lambda)$ can be restored.

Of course, Eq. (5) 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. (5) 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. (5) and (6)].

The wave forms of the two simplest functions for N=4,6 [N should be even in Eq. (6)] are presented in Fig. 1. The best signal-to-noise ratio was obtained for very wide strobes with widths equal to the distance between them.

The most important feature of the new weighting functions is that they provide narrow-band filters with nearly symmetrical characteristics. Even the simplest four-step filter GS-4 has better resolution than the more complicated filter of the fourth order HiRes-5[5] (see also Ref. 9). Filter GS-6 yields a resolution as high as $w \sim 3.4$. This value is more than two times better than the resolution limit ($w \approx 4.4$) of traditional correlation DLTS, estimated in Ref. 9. 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 $\mathrm{SNR}^{-1} = \mathrm{N/S} \approx 900$ (S is given by the ratio of the output DLTS signal to the amplitude of exponential transient at the input of the correlator; N is the measure of the amplification of noise by the correlator and was calculated using a formula from Refs. 3 and 13). 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 $N_T/N_D = 2\Delta C/C \sim 0.2 - 0.02$. Therefore, this weighting function may be employed for the analysis of intensive peaks in spectra in temperature-scanned DLTS.

Weighting functions obtained from the Gaver–Stehfest algorithm for higher values of N provide better resolution (for example, $w = 2.67$ for $N = 8$ and $w = 2.27$ for $N = 10$), but require such a high signal-to-noise ratio of the transient that they can be employed only for decays, obtained by averaging thousands of transients at fixed temperature (as is usually done for inverse Laplace DLTS[14]).

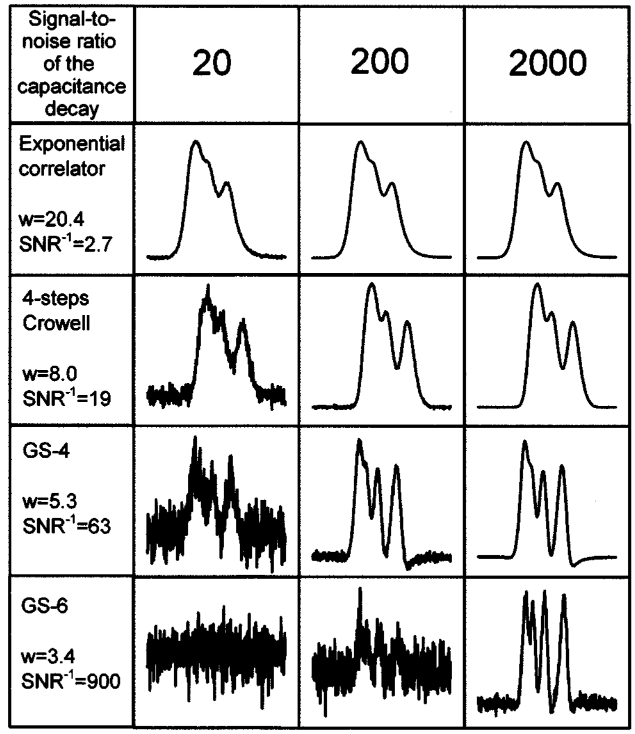

FIG. 2. DLTS spectra, simulated with different levels of Gaussian-distributed noise in capacitance decays for the system of four closely adjacent levels ($E_a = 0.4$, 0.425, 0.465, 0.53 eV, $\sigma = 10^{-14}\ \mathrm{cm}^2$) and correlated with different weighting functions. The decrease in DLTS peak width from $w = 20.4$ (exponential correlator) to $w = 3.4$ (GS-6) permits the resolution of all four levels. A good estimate for the maximum noise level in the input capacitance decay, which is required to employ the weighting function without averaging of transients, is given by $\boldsymbol{SNR}^{-1} = \mathrm{N/S}$, where S is the DLTS signal, determined from Eq. (1) at the DLTS maximum, N is the noise level, found from the formula given in Refs. 3 and 5.

III. DISCUSSION AND CONCLUSIONS

With the development of inexpensive fast desk-top computers, it has become easier and cheaper to digitize capacitance transients and correlate them numerically than to use expensive analog correlators. In an automated setup, one can easily process the same transients with different correlation functions (corresponding to different rate windows or different resolution capacity). Therefore, a proper choice of the correlation function becomes a powerful (and the least expensive) tool to achieve better resolution in DLTS. The DLTS peak width of $w \sim 3$, which can be reached using properly chosen correlation functions, is comparable to the value of $w \sim 2$, which was obtained[14] using numerical inversion of the Laplace integral equation.

The weighting functions, based on the Gaver–Stehfest algorithm, represent a new class of narrow-band filters and allow us to obtain resolution as high as $w \approx 3.4$, for high, but a still-realistic signal-to-noise ratio of the input transient of about 900. This is equivalent to a three-times gain in the energy resolution as compared to the standard double boxcar, and can be reached without considerable programming effort.

In order to provide a clear example of the limitations in resolution of standard weighting functions, compare them with the resolution of Gaver–Stehfest correlation functions and get an idea of the sensitivity of different weighting functions to noise, DLTS spectra of four closely spaced deep levels were simulated. First, capacitance decays corresponding to the emission from four deep levels ($E_a = 0.400$; 0.425; 0.465; 0.530 eV, $\sigma = 1 \times 10^{-14}\ \mathrm{cm}^{-2}$) were simulated for temperatures between 100 and 300 K with a step of 0.5 K. Then, Gaussian-distributed noise [signal-to-noise ratio (SNR) of the transients was 20, 200, and 2000] was added and the transients were correlated with different weighting functions. The resulting DLTS spectra are presented in Fig. 2. As expected, the exponential correlator[2] has a very good tolerance to noise in the input signal and, unlike the other three simulated correlators, provides an excellent DLTS spectrum even for SNR=20. However, it cannot resolve the structure of decay—the first two peaks are merged, and the third one appears as a ledge on the background of the summary peak due to the first two.

The four-step function of Crowell,[3] which belongs to third-order filters, gives a noisy spectrum for SNR=20, but works well for higher signal-to-noise ratios. It allows us to isolate the third peak much better than the exponential correlator, but the first two levels stay unresolved. The double structure of the first DLTS peak is clearly seen if one uses the Gaver–Stehfest function GS-4, and can be resolved completely by GS-6, which, however, requires a signal-to-noise ratio of more than a thousand.

The idea, frequently appearing in the literature, that in principal the resolution of correlation spectroscopy is limited compared to more sophisticated methods of the inverse Laplace transform, proves to be wrong. The introduction of Gaver–Stehfest weighting functions as filters for correlation spectroscopy means that there is no substantial difference between correlation spectroscopy and methods of inversion of the Laplace integral equation. The distance between the energies of the two deep levels of 25 meV, which was the typical distance between the components of the DX center, resolved by the method of Tikhonov's regularization in Ref. 14, can be successfully resolved by correlation spectroscopy as well (Fig. 2). The main criterion to prefer on weighting function to another should be the effectiveness of each concrete method, i.e., its capability to provide the best resolution with the lowest input signal-to-noise ratio.

ACKNOWLEDGMENTS

The author is particularly indebted to O. F. Vyvenko for longstanding discussions on capacitance spectroscopy, which stimulated the appearance of this article. Overall support by E. R. Weber, critical remarks on the manuscript made by E. Edelson, E. E. Haller, H. Hieslmair, and V. M. Ustinov are gratefully acknowledged. This work was supported by NREL Subcontract No. XD-2-11004-3.

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