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In this article, a modified covariance method for analyzing deep-level transient spectroscopy (DLTS) capacitance transients using a combined singular value decomposition/Prony (SVD–Prony) method is presented. This combined method is based upon using the SVD method first to accurately estimate the number of exponentials contained in transient capacitance data, then the Prony method is applied to obtain an accurate estimate of the exponential time constants. Results are presented for simulated exponential data with additive white-Gaussian noise and for real DLTS data to demonstrate the applicability of the presented technique. In addition, a statistical analysis is performed to study the behavior of this technique and its effectiveness in extracting the capacitance parameters at different noise levels. Finally, the problem of multiple exponential detection is addressed. © *1998 American Institute of Physics.* [S0034-6748(98)05006-0]

I. INTRODUCTION

Introduced first by Lang,[1–3] deep-level transient spectroscopy (DLTS) is a semiconductor characterization method that has been widely used to study deep levels in semiconductors. However, one of the drawbacks of Lang's technique is the inability to distinguish between two or more closely spaced defect levels. This was overcome by techniques that fall into two general categories.[4] The first group includes techniques such as correlation[5] and spectral fitting.[6,7] This group involves the direct analysis of the DLTS spectrum. The second group involves the estimation of parameters associated with capacitance transients. These include methods such as linear predictive modeling,[8] figure of merit,[9] fast Fourier transform[10] method of moments,[11] and modulation function.[12]

Most correlation techniques[5] use the method of cross correlation to extract the capacitance transient parameters. However, these methods are very sensitive to additive noise and also fail to distinguish between two closely spaced defect levels. Other methods, such as the deep-level transient Fourier spectroscopy,[10] have been shown to permit highly accurate parameter estimation. The spectral fitting methods, such as single scan deep-level transient spectroscopy,[7] are capable of analyzing overlapping signals; however, they have the inherent disadvantage of needing a large number of variables to fit the spectrum. The method of moments[11] calculates the exponential parameters from the time-weighted integrals of the measured response, but is very sensitive to noise. Covariance methods, such as covariance linear predictive modeling (CLPM),[8] use matrix decomposition techniques to estimate the exponential capacitance parameters. However, the performance of CLPM techniques must be scrutinized in the presence of noise.

In this article, a hybrid technique related to CLPM for analyzing DLTS systems is presented. The technique is based on a combined singular value decomposition (SVD)[13]/Prony[14] method, where the SVD method is used first to accurately estimate the number of exponentials contained in transient capacitance data, then the Prony method is applied to obtain an accurate estimate of the exponential time constants. It is known that the SVD–Prony method is a robust technique for estimating the parameters of exponentially damped sinusoids (i.e., data with complex poles).[15] In this report we exploit the purely exponential transients (i.e., strictly real poles) encountered in DLTS to simplify the singular value decomposition and thus improve order estimation. Results are presented for simulated exponential data with additive white-Gaussian noise at different noise levels and for real DLTS data to demonstrate the applicability of the presented technique. We will show that the SVD–Prony method is effective at estimating time constants from data and for testing the transient for multiple exponentials at signal-to-noise ratios (SNR) as low as 6 dB.

II. SVD–PRONY METHOD

A. Formulation

In general, capacitance transients can be modeled as a linear combination of exponentials, i.e.,

$$c(n)=C_0+\sum_{i=1}^{P} C_i z_i^n + w(n), \quad n=0,1,...,N-1, \tag{1}$$

where C_0 is the base-line capacitance; C_i is the ith capacitance amplitude; P is the system order; i.e., the number of exponentials present in the data; N is the data length; $w(n)$ is an additive noise sequence; and

$$z_i=e^{-\frac{\tau_s}{\tau_i}}, \tag{2}$$

with τ_i and τ_s being the ith defect time constant and the sampling time, respectively.

As demonstrated by Kumaresan and Tufts,[13] the use of the singular value decomposition can provide a robust estimation procedure. In matrix notation, the SVD approach begins with the recursive difference equation

$$\mathbf{\Phi}_L \mathbf{B}_L = -\mathbf{C}_L, \tag{3}$$

where

$$\mathbf{\Phi}_L = \begin{bmatrix} c_{L-1} & c_{L-2} & \cdots & c_0 \\ c_L & c_{l-1} & \cdots & c_1 \\ \vdots & c_{N-3} & \cdots & \vdots \\ c_{N-2} & & & c_{N-L-1} \end{bmatrix}, \tag{4}$$

$$\mathbf{C}_L = [c_L \quad c_{L+1} \quad \cdots \quad c_{N-1}]^T, \tag{5}$$

and

$$\mathbf{B}_L = [b_0 \quad b_1 \quad \cdots \quad b_L]^T. \tag{6}$$

Here, $\mathbf{\Phi}_L$, $\mathbf{C}_L$, and $\mathbf{B}_L$ are the data matrix (Toeplitz structure), data coefficient vector, and coefficient vector whose elements are related to the defect time constants, respectively. Note that an overdetermined system order L is used, i.e., $P < L \leqslant N/2$ and it is recommended to choose $L \leqslant N/3$ for best results.[13]

The SVD technique is used first to decompose $\mathbf{\Phi}_L$ such that

$$\mathbf{\Phi}_L = \mathbf{U}\mathbf{S}\mathbf{V}^T = \sum_{i=1}^{L} \sigma_i \mathbf{u}_i v_i^T, \tag{7}$$

where $\mathbf{U}$ and $\mathbf{V}$ are unitary matrices whose columns are formed from the eigenvectors of $\mathbf{\Phi}_L \mathbf{\Phi}_L^T$ and $\mathbf{\Phi}_L^T \mathbf{\Phi}_L$, respectively, and $\mathbf{S}$ is a rectangular matrix whose diagonal elements are the singular values σ_i, $\{i = 1,2,...,L\}$ with $\sigma_i^2 = \lambda_i$, λ_i is the ith eigenvalue of the real symmetric matrix $\mathbf{\Phi}_L^T \mathbf{\Phi}_L$. The actual number of exponentials corresponds to the number of nonzero singular values.

Since the number of exponentials P is unknown, then the singular values can be used to obtain an estimate of P by ordering the singular values from the largest to the smallest. The order estimate is then obtained by locating the largest gap occurring between two successive singular values. Thus,

$$\sigma_1 > \sigma_2 > \cdots > \sigma_P > \sigma_{P+1} > \cdots > \sigma_L, \tag{8}$$

with $\sigma_{p+1},...,\sigma_L$ set to zero. Using the truncated form for Eq. (7), i.e.,

$$\Phi_L \approx \sum_{i=1}^{P} \sigma_i u_i v_i^T, \tag{9}$$

and the unitary properties of $\mathbf{U}$ and $\mathbf{V}$, yields an approximation of the coefficient vector $\mathbf{B}_L$,

$$\mathbf{B}_L \approx \sum_{i=1}^{P} \frac{-1}{\sigma_i} \mathbf{v}_i \mathbf{u}_i^T \mathbf{C}_L. \tag{10}$$

The elements of the coefficient vector $\mathbf{B}_L$ are then used to obtain the corresponding defect time constants, base-line capacitance, and capacitance amplitudes via the Prony method.[14]

B. Noise effects

The singular value decomposition is a powerful tool to measure the sensitivity of the parameter estimates when the data are subject to noise perturbations. In cases where the number of exponentials is unknown, the SVD method can be effectively used to select the appropriate order by comparing the relative magnitudes of the singular values. If there is no noise in the data, the SVD technique yields an exact order estimate since only P singular values are nonzero. With the presence of additive noise, the eigenvalues are perturbed by fluctuations with variance $(N\text{-}L)\sigma_w^2$, with σ_w^2 being the noise variance. Thus, truncating the sum in Eq. (7) at the proper order reduces the noise contributions and provides a minimum norm approximation. Generally, for moderate noise content, the noise-induced singular values are significantly smaller than the singular values from the signal. This makes the order selection relatively simple and, consequently, the number of the larger singular values is an estimate of the number of exponentials. For data with low SNR, the noise singular values are, in general, comparable in magnitude to the signal singular values, and the truncation based on the relative magnitude of the singular values is no longer appropriate to use.

III. APPLICATIONS TO DLTS SYSTEMS

A. SVD truncation

In general, the estimation of the number of exponentials depends upon the separation of the singular values. For the complex exponential model, many criteria have been proposed to truncate the SVD at the appropriate order for low SNR.[16,17] Some require *a priori* knowledge of the noise variance,[16] which is impractical. Others require solving nonlinear equations where the computation becomes intensive.[17]

Based on the properties of DLTS data, a selection criterion is more easily developed. After rearranging the singular values in descending order, from the largest to the lowest, as in Eq. (8), this criterion consists of systematically increasing the order, starting from order 1, and monitoring the locations of the roots of the polynomial formed from the coefficient vector $\mathbf{B}_L$. The optimum order is then obtained by employing the following criteria:

(1) Eliminate all complex roots, since they are not compatible with the model of Eq. (1), which is in turn derived from physical principals.[1]

(2) Eliminate all negative real roots, since they cause the system to be unstable and are not physically possible.

B. Single-exponential estimation

To illustrate the use of the presented formulation, simulated single-exponential noisy data are considered. The selected signal component is

$$C(n) = C_0 + C_1 e^{-n\tau_s/\tau_1}, \tag{11}$$

where $C_0 = 20$, $C_1 = 30$, $\tau_s = 1$ ms, and $\tau_1 = 2$ ms. The simulation uses 680 data samples (consistent with the experimental data discussed in the next section) and the additive noise is a zero-mean white-Gaussian process. The SVD–Prony al-

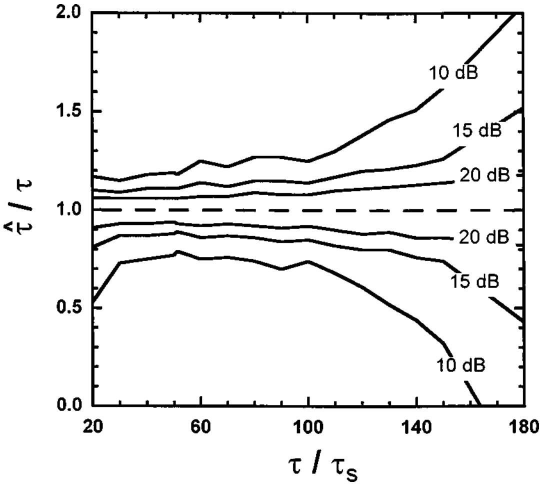

FIG. 1. SVD–Prony algorithm performance for SNR values of 10, 15, and 20 dB.

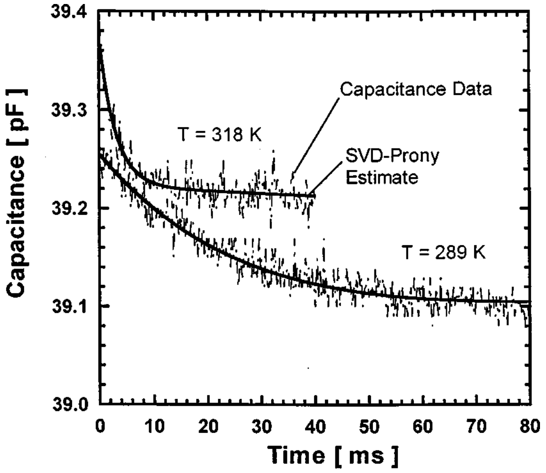

FIG. 3. Capacitance transients observed using trap analysis on characterization system (TACs).

gorithm coded in MATLAB is then applied to the single-exponential simulated data at signal-to-noise ratios of 20, 15, 10, and 6 dB. Here, the SNR is defined as

$$\mathrm{SNR} = 10 \log_{10} \frac{1}{\sigma_w^2}. \tag{12}$$

A statistical analysis in terms of a 95% confidence interval is then performed to study the behavior of the foregoing technique. Figures 1 and 2 illustrate the performance of our SVD–Prony algorithm at different SNR values with τ/τ_s ranging from 20 to 180. It is clear from Figs. 1 and 2 that the SVD–Prony method can accurately estimate the exponential time constant even with a SNR value of 6 dB over a limited τ/τ_s range.

C. Analysis of experimental capacitance transients

Capacitance transients from a 6H–silicon–carbide diode are now analyzed using the SVD–Prony algorithm to demonstrate the usefulness of the algorithm for application to deep-level transient spectroscopy. Capacitance transients were measured on a 6H–SiC *pn*-junction diode grown using chemical vapor deposition. The details of diode fabrication and the identification of the room-temperature minority-carrier DLTS spectrum as the *D* center are described in Ref. 18. It is sufficient to note here that the sample is a two-sided abrupt-junction diode with a nitrogen-doped *n*-type layer and an aluminum-doped *p*-type layer symmetrically doped to background densities of 3×10^{15} cm^{-3} each. The minority-carrier trap-filling pulse produced a 2.55 V forward bias on the diode, and the injection current during the pulse was approximately 6 mA. The capacitance transient was observed at a static bias of -15 V. We confirmed that the 10 μs trap filling pulse width was sufficient to fill the *D*-center hole trap.[19]

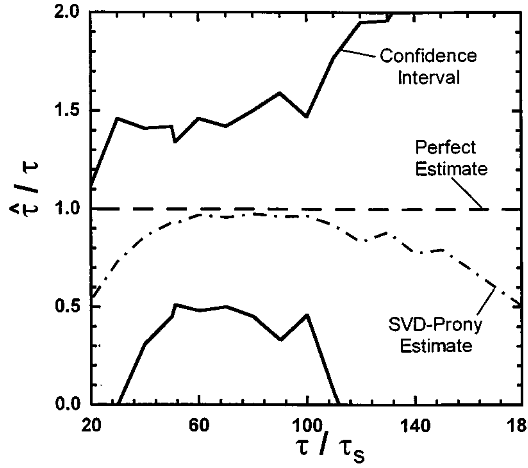

FIG. 2. SVD–Prony algorithm performance for a SNR value of 6 dB.

Figure 3 illustrates two capacitance transients digitized from this diode at two different temperatures (288 and 318 K). The capacitance transients were digitized with a Hewlett Packard (HP) 4280 A capacitance versus time plotter. The transients were digitized at the same sampling interval of 200 μs. The length of the data record was increased to accommodate the longer time constants observed at progressively lower temperatures. The wave forms in Fig. 3 represent single-shot captures of the transients (i.e., no wave-form averaging). The data, following capture by the HP 4280 A, was transferred to a personal computer for postprocessing.

The transients, on first glance, appear to be likely candidates for modeling with the classic DLTS single-exponential model of Eq. (11). The transients were analyzed using the previously described SVD–Prony algorithm coded in the MATLAB Unix environment. The order estimated by the SVD–Prony algorithm was 2, with the first time constant being very long compared to the sampling time ($\tau/\tau_s > 10^5$), which we interpret as a constant. The second time constant for each transient in Fig. 3 was estimated by the algorithm to be 26 and 3.0 ms for the 288 and 318 K transients, respectively. The solid lines drawn through the data in Fig. 3 represent Eq. (1) employing the algorithm's parameter estimates. An estimate of the signal-to-noise ratio for both wave forms was determined by subtracting Eq. (1) from the time series representing the digitized data, and then computing the noise variance using the histogram method. The time series representing the noise were normalized with the esti-

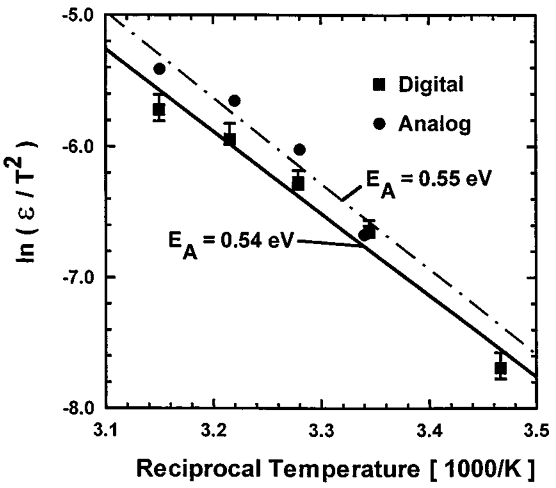

FIG. 4. Arrhenius plot comparing TACS digital data analysis with conventional analog DLTS system performance.

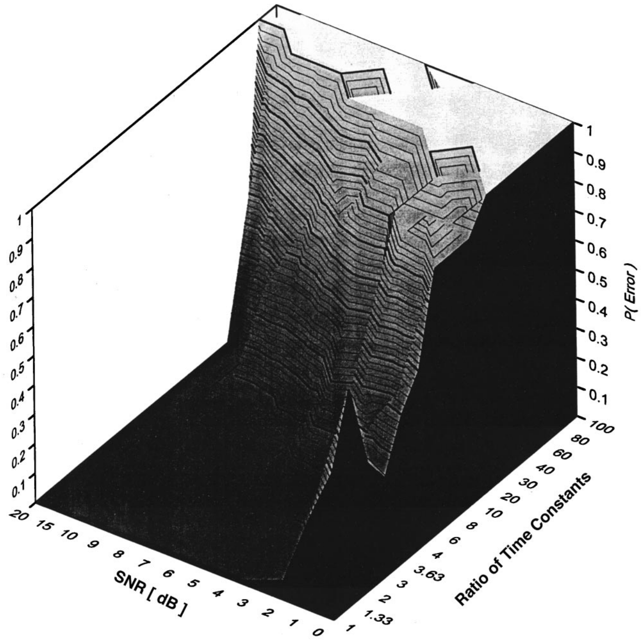

FIG. 5. SVD–Prony algorithm performance for multiple exponential detection.

mates of the peak amplitudes of the exponential transients (i.e., ΔC). The estimated SNR is 23 dB for the $T=289$ K wave form in Fig. 3, and 20 dB for the $T=318$ K wave form in Fig. 3.

Transients at three other temperatures where digitized and processed with the SVD–Prony algorithm. Using the estimated time constants, an Arrhenius plot was formed using the widely held assumption that the capture cross section varies with the reciprocal of the square of the temperature ($\sigma \propto T^{-2}$). Figure 4 contains this plot along with error bars computed using the 20 dB confidence intervals from Fig. 1. For comparison, data are plotted from an independent measurement on the same diode under virtually identical forward bias injection conditions using an analog DLTS system (utilizing a correlation filter matched to a single-exponential wave form). These results were first reported in Ref. 18. Clearly, the activation energies, as indicated in Fig. 4, are, within the statistical significance of the measurement, virtually identical. Thus, the SVD–Prony algorithm has been shown to be a useful processing option for performing classic DLTS measurements on *pn* diodes.

IV. MULTIPLE EXPONENTIAL DETECTION

We conclude with a word on the testing of the single-exponential hypothesis. By assuming a single-exponential model, analysts of deep-level transient spectroscopy data often neglect the fact that multiple-exponential models may physically occur. One common example is the use of a filter matched to a single-exponential transient in the analog or digital correlator. In the literature, there are methods reported for testing the single-exponential hypothesis, such as the ‘‘simple’’ Diophantine test by Batovski and Hardalov.[20] The Diophantine test is applicable to either conventional analog DLTS or to digital capacitance–transient capture that is analyzed in the conventional manner (i.e., Lang’s approach). We have applied the Diophantine test on the capacitance transients shown in Fig. 3, but the signal-to-noise ratio, even at 20 dB, was insufficient to give reliable results. In fact, the principal weakness of the Diophantine test as presented in Ref. 20 is the lack of criteria for rejecting the single-exponential hypothesis. In contrast, the SVD–Prony algorithm performs a nearly perfect test of the single-exponential hypothesis under these conditions, as is demonstrated shortly.

Doolittle and Rohatgi focus on the resolution of multiple deep centers, rather than on nonexponential transient detection.[4,21] In this approach, resolution is defined in terms of the smallest difference in energy between two deep levels that the DLTS system can detect. Doolittle and Rohatgi avoid confusion introduced by unnecessary data processing, such as computing the classic DTLS spectrum, by concentrating on the resolution of two exponential time constants, an approach we repeat here. Nevertheless, their figure of merit L confuses the distinction between what a DLTS system measures (a capacitance transient) and the physical interpretation of the data, which is based on an assumed physical model.

The SVD–Prony algorithm reported here permits the appropriate order of the model to be suggested by analysis of the data prior to parameter estimation, and thus represents a significantly more general approach to performing deep-level transient spectroscopy than was previously possible with hardware-specific signal processing (e.g., analog systems employing filters implemented in hardware). In particular, we have tested the performance of the SVD–Prony algorithm at detecting multiple-exponential transients (in the form of the sum of two exponential transients), and thus the results are directly applicable to the measurement process without unnecessary reference to the physical interpretation process. The performance of the SVD–Prony method was determined with simulated transient data consisting of two time constants of finite separation with additive white noise. The simulated data satisfies the linear model of Eq. (1), with $P=2$, $C_0=0$, $C_1=3$, $C_2=5$, $\tau_2/\tau_s=80$, and $N=680$. Multiple trials of the SVD–Prony algorithm with the simulated data were performed at various signal-to-noise ratios and various discrete values of τ_1/τ_2 ranging from 1 to 100.

In Fig. 5, the performance of the algorithm at multiple-exponential detection is indicated by a normalized histogram of errors (an error is defined as an order estimate other than 2) after n trials (typically, $n=100$, except near the extremes of the distribution, where $n=20$); thus, the surface plotted in Fig. 5 represents an estimate of the joint probability distribution function for making an error in detecting two time constants as a function of τ_1/τ_2 and the signal-to-noise ratio. The most common error was detecting only one of the two time constants, similar to that reported in Ref. 21 for the related technique of the covariance method of linear predictive modeling.

In this article, we make no claim about the accuracy of multiple time constant *estimation* (as opposed to *detection*), which will be the subject of a future paper. Also, this preliminary result strictly applies only to DLTS transients formed by the sum of two exponentials with nearly equal magnitude and the specified time-constant ratios. Clearly, the case of two exponentials with greatly differing magnitudes is physically likely, but undocumented here. Still, Fig. 5 illustrates that the algorithm is effective at testing the single-exponential hypothesis at signal-to-noise ratios greater than 5 dB and time constants differing by less than an order of magnitude. In practice, both conditions represent physically relevant scenarios.

V. DISCUSSION

A combined SVD–Prony method has been successfully applied to DLTS capacitance transients. This technique, in addition to being a robust estimator, is shown to be effective in extracting exponential parameters associated with DLTS data at signal-to-noise ratios as low as 6 dB. The performance of this method is evaluated in terms of the 95% confidence interval for different noise levels. Furthermore, it is shown that this technique is effective not only in testing the single-exponential hypothesis, but also in detecting multiple-exponential models.

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