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LINESHAPE ANALYSIS FOR CAPACITANCE TRANSIENT SPECTRA. (U)
SEP 79 J T SCHOTT
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20. ABSTRACT (Continue on reverse side if necessary and identify by block number) → The capacitance transient spectroscopic technique is described along with the major variations in the techniques depending on the particular instrumentation used to process the capacitance transient. Expressions for the theoretical line shape are derived for the lock-in amplifier version of the technique with arbitrary phase setting. The results show excellent agreement with experimental spectra. Expressions are derived which are useful in determining defect level parameters from a single spectrum, rather than from an			

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20. Abstract (Continued)

Arrhenius plot from a series of spectra. A computer program is given for plotting theoretical spectra, which is useful for determining the effects of defect level parameters on spectra and for unfolding complex spectra.

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Contents

1. INTRODUCTION	5
2. SIMPLIFIED LOCK-IN AMPLIFIER TREATMENT	7
3. MORE EXACT TREATMENT FOR 0° PHASE	8
4. LINESHAPE FOR ARBITRARY PHASE	9
5. DETERMINATION OF ACTIVATION ENERGY FROM LINESHAPE	11
REFERENCES	17
APPENDIX: Computer Plotted Spectra	19

Illustrations

1. Theoretical Lineshapes for the Lock-In Amplifier Version of Capacitance Transient Spectroscopy for Different Lock-In Amplifier Phase Settings (Mixer 0° or 24.5° Before Beginning of Capacitance Transient) or for Phase Independent (Vector Amplitude) Output	12
2. Experimental Spectra for the E-Center in Electron Irradiated Silicon for Two Lock-In Amplifier Phase Settings	12

Table

1. Lineshape Expressions and Values of Parameters Defined in the Text, for Various Lock-In Amplifier Phase Settings

15

Lineshape Analysis for Capacitance Transient Spectra

1. INTRODUCTION

Capacitance transient spectroscopy has, in recent years, gained widespread use in the detection and study of defect states in semiconductor materials and devices.¹ The technique was originally developed by Lang² and called deep-level transient spectroscopy (DLTS). Major variations on the technique have been developed by Kimerling³ and Miller et al.⁴

The technique is based on the work of Williams⁵ and Sah et al⁶ where a transient is produced in the capacitance of a diode structure, following a sudden bias increase, and resulting from charge carrier emission from defects in the depletion region. Determination of the decay-time constant, τ , of the capacitance transient as a function of temperature yields important information about the defect centers.

(Received for publication 1 November 1979)

1. Miller, G. L., Lang, D. V., and Kimerling, L. C. (1977) Ann. Rev. Mat. Sci. 1977:377.
2. Lang, D. V. (1974) J. Appl. Phys. 45:3023.
3. Kimerling, L. C. (1977) Radiation effects in semiconductors - 1976, Inst. of Physics Conf. Series No. 31, 221.
4. Miller, G. L., Ramirez, J. V., and Robinson, D. A. H. (1975) J. Appl. Phys. 46:2638.
5. Williams, Richard (1966) J. Appl. Phys. 37:3411.
6. Sah, C. T., Forbes, L., Rosier, L. L., and Tasch, Jr., A. F. (1970) Solid-State Electron. 13:759.

In capacitance transient spectroscopy, periodic bias pulses are used to produce a repetitive train of capacitance transients. This signal is then processed by some apparatus which has a peak response for a particular τ . As the temperature of the sample is varied, a peak in the output of this apparatus will be recorded each time the emission-time constant of a defect matches that to which the instrument is tuned. The lineshape of the spectra which are obtained depend on the particular apparatus used to process the capacitance transient signal. Lang² used a double boxcar integrator. Kimerling³ uses a lock-in amplifier. Miller⁴ uses an exponential correlator. The paper by Miller et al⁴ gives the lineshape for the double boxcar and exponential correlator, and also for one particular phase setting of a lock-in amplifier.

Different phase settings are possible when using a lock-in amplifier due to the way it processes the capacitance transient signal. The tuned amplifiers of the input channel allow only the fundamental Fourier component of the signal to pass. The mixer then passes the signal unaltered for a half cycle and inverts the next half cycle. It is the phase of this operation which is adjustable. Finally, the output filters smooth this out to a D. C. average output. The phase of the fundamental Fourier component is not constant in our case, since as temperature is varied, the time constant of the exponential decay varies, resulting in a variation of the phase of the signal reaching the lock-in mixer.

If the mixer operation phase is set to coincide with the beginning of the capacitance transient (end of the bias pulse) then one gets the lineshape reported by Miller et al.⁴ However, if the phase is set to be in phase with the fundamental Fourier component at that temperature for which it has maximum amplitude, then a different lineshape is generated. Some lock-in amplifiers have a phase independent (vector amplitude) output which gives still another lineshape.

In previous work^{7, 8} we have used the second mentioned phase setting, choosing to be in phase with the fundamental Fourier component at maximum amplitude of this component. This has been shown⁹ to require a phase setting of 24.5° before the bias pulse (beginning of transient). This phase setting is convenient since one can monitor the mixer output during a run and verify that the in-phase point occurs at the peak in the output. This gives assurance that the lock-in amplifier has been properly tuned and has not drifted, which can be a concern at very low frequencies (down to 0.2 Hz).

7. Drevinsky, P.J., Schott, J.T., DeAngelis, H.M., Kirkpatrick, A.R., and Minnucci, J.A. (1979) Conf. Record of the Thirteenth IEEE Photovoltaics Specialists Conference - 1978, 1232.
8. Schott, J.T., DeAngelis, H.M., and Drevinsky, P.J. (1980) J. Electron. Mat., to be published.
9. Schott, J.T., DeAngelis, H.M., and White, W.R. (1976) Air Force Technical Report, AFCRL-TR-76-0024.

In a previous report⁹ we derived the expressions necessary to relate lock-in amplifier frequency to emission time constant and peak height to defect concentration, for this phase setting. Each time a spectrum at a different frequency is generated, another time constant/temperature data point for an Arrhenius plot which will yield the basic defect parameter is received. However, this only uses one point of each spectrum, namely, the peak position. The rest of the lineshape contains information about the emission time constant at other temperatures as well. In fact a single spectrum at a single frequency contains all the information necessary to obtain the parameters received from an Arrhenius plot using a number of spectra at different frequencies.

In this report, we derive the theoretical lineshape for arbitrary lock-in amplifier phase, and the expressions necessary to extract information from these spectra. Theoretical curves are compared with experimental spectra. An appendix gives a computer program to generate theoretical capacitance transient spectra.

2. SIMPLIFIED LOCK-IN AMPLIFIER TREATMENT

A simplified view of lock-in amplifier operation is to consider it to act as a correlator with a sine wave weighting function. This is the view taken by Miller et al⁴ in comparing the lock-in approach with their exponential correlator approach. Then for a capacitance signal of the form $\exp(-t/\tau)$, we get a lock-in response of the form

$$A = \frac{1}{L} \int_0^L e^{-t/\tau} \sin \frac{2\pi t}{L} dt \quad (1)$$

$$= \frac{2\pi(1 - e^{-L/\tau})}{\frac{L}{\tau^2} + 4\pi^2} \quad (2)$$

where the lock-in amplifier is tuned to a frequency, $F = 1/L$. If we define a dimensionless parameter, α , such that

$$\alpha = \frac{\tau}{L} = \tau F \quad (3)$$

we then get the lineshape expression

$$A(\alpha) = \frac{2\pi\alpha^2(1 - e^{-1/\alpha})}{4\pi^2\alpha^2 + 1} \quad (4)$$

Of course A is implicitly a function of temperature T, through the standard emission rate equation

$$\alpha = \tau F = F \frac{e^{\Delta E/kT}}{\sigma \langle v \rangle N} \quad (5)$$

where k is the Boltzmann constant, σ is the defect capture cross section, $\langle v \rangle$ is the carrier thermal velocity, and N is the density of states of the appropriate band. This lineshape is the one reported by Miller et al⁴ for Kimerling's lock-in amplifier spectra.

3. MORE EXACT TREATMENT FOR 0° PHASE

For a more careful treatment, we must consider the complete sequence of input channel filtering, mixing, and output channel filtering. The effect of the tuned amplifiers of the input channel is to pass only the fundamental Fourier component of the exponential train. In a previous report,⁹ we showed this Fourier component to be

$$F(t) = a_1 \cos \frac{2\pi t}{L} + b_1 \sin \frac{2\pi t}{L} \quad (6)$$

$$= c_1 \sin \left(\frac{2\pi t}{L} + \tan^{-1} \frac{a_1}{b_1} \right) \quad (7)$$

where

$$a_1 = \frac{2\alpha(e^{-1/\alpha} - 1)}{(4\pi^2\alpha^2 + 1)} \quad (8)$$

$$b_1 = \frac{4\pi\alpha^2(e^{-1/\alpha} - 1)}{(4\pi^2\alpha^2 + 1)} \quad (9)$$

$$c_1 = \frac{2\alpha(e^{-1/\alpha} - 1)}{(4\pi^2\alpha^2 + 1)^{1/2}} \quad (10)$$

$$\frac{a_1}{b_1} = \frac{1}{2\pi\alpha} \quad (11)$$

The effect of the mixer operation and the averaging of the output channel filters can then be given by

$$A = \frac{1}{L} \int_{-L/2}^0 F(t) dt - \frac{1}{L} \int_0^{L/2} F(t) dt \quad (12)$$

provided the phase of the mixer operation is set to 0 degrees with respect to the beginning of the capacitance transient. Substituting for the Fourier component using Eq. (6), we find that the cosine term averages to zero, and we are left with

$$\begin{aligned} A(\alpha) &= b_1 \left\{ \frac{1}{L} \int_{-L/2}^0 \sin \frac{2\pi t}{L} dt - \frac{1}{L} \int_0^{L/2} \sin \frac{2\pi t}{L} dt \right\} \\ &= b_1 \left\{ -\frac{2}{\pi} \right\} = \frac{8\alpha^2(1 - e^{-1/\alpha})}{4\pi^2\alpha^2 + 1} \quad (13) \end{aligned}$$

Note that this is of the same form as Eq. (4) found above, only differing by a constant factor.

4. LINESHAPE FOR ARBITRARY PHASE

The above lineshape is only correct for a particular phase setting of the lock-in amplifier. As mentioned in the introduction, however, other phase settings are sometimes convenient. If we consider the lock-in mixer operation phase to be set to an arbitrary angle ϕ ($0 \leq \phi \leq 2\pi$) before the beginning the capacitance transient, then the lock-in reponse will be given by

$$A = \frac{1}{L} \int_{(-L/2 - \phi L/2\pi)}^{-\phi L/2\pi} F(t) dt - \frac{1}{L} \int_{-\phi L/2\pi}^{(L/2 - \phi L/2\pi)} F(t) dt \quad (14)$$

Substituting for the Fourier component from Eq. (7) we have

$$\begin{aligned} A &= c_1 \left\{ \frac{1}{L} \int_{(-L/2 - \phi L/2\pi)}^{-\phi L/2\pi} \sin \left(\frac{2\pi t}{L} + \tan^{-1} \frac{1}{2\pi\alpha} \right) dt \right. \\ &\quad \left. - \frac{1}{L} \int_{-\phi L/2\pi}^{(L/2 - \phi L/2\pi)} \sin \left(\frac{2\pi t}{L} + \tan^{-1} \frac{1}{2\pi\alpha} \right) dt \right\} \\ &= c_1 \left\{ -\frac{2}{\pi} \cos \left(\tan^{-1} \frac{1}{2\pi\alpha} - \phi \right) \right\} \end{aligned} \quad (15)$$

Thus, substituting Eq. (10), we have

$$A(\alpha) = \frac{4\alpha(1 - e^{-1/\alpha})}{\pi(4\pi^2\alpha^2 + 1)^{1/2}} \cos \left(\tan^{-1} \frac{1}{2\pi\alpha} - \phi \right) \quad (16)$$

We can now consider some special cases. For $\phi = 0$, we can construct a right triangle with two sides of length 1 and $2\pi\alpha$, and by calculating the hypotenuse, immediately find

$$\cos \left(\tan^{-1} \frac{1}{2\pi\alpha} \right) = \frac{2\pi\alpha}{(4\pi^2\alpha^2 + 1)^{1/2}} \quad (17)$$

Making this substitution, we get the lineshape of Eq. (13) found above.

In a previous report⁹ we found the value of α , to be denoted α_{\max} , for which the amplitude of the fundamental Fourier component (coefficient c_1 given by Eq. (10)), is a maximum. To be in phase with the Fourier component at its maximum amplitude, we must set the lock-in phase to

$$\phi = \tan^{-1} \frac{1}{2\pi\alpha_{\max}} \cong 24.5^\circ$$

The lineshape is then

$$A(\alpha) = \frac{4\alpha(1 - e^{-1/\alpha})}{\pi(4\pi^2\alpha^2 + 1)^{1/2}} \cos \left(\tan^{-1} \frac{1}{2\pi\alpha} - 24.5^\circ \right) \quad (18)$$

This is the lineshape appropriate for all our published data.

If one has a lock-in amplifier which has a phase independent or vector amplitude output, then the lineshape is just the general form without the cosine factor

$$A(\alpha) = \frac{4\alpha(1 - e^{-1/\alpha})}{\pi(4\pi^2\alpha^2 + 1)^{1/2}} \quad (19)$$

Such instruments are really dual channel lock-in amplifiers with one channel output related to the cosine of the phase angle as above, and the other channel 90° out of phase and related to the sine of the phase angle. The phase independent or vector amplitude output is obtained from the sum of the squares of these two outputs.

Figure 1 shows a plot of each of the three lineshape equations plotted on a temperature scale appropriate for the thermocouple used in our experiments. The curves are generated by using Eq. (5) to determine the value of α for each temperature value, and then using the appropriate $A(\alpha)$ equation to determine the amplitude at that temperature. Figure 2 shows experimental spectra for two different phase settings. The agreement between theory and experiment is excellent.

5. DETERMINATION OF ACTIVATION ENERGY FROM LINESHAPE

In the introduction, it was pointed out that a single spectrum contains all the information necessary to determine the defect activation energy, provided more than just the peak maximum point is used. From Eq. (5) we can write

$$\alpha = C T^{-2} e^{\Delta E/kT} \quad (20)$$

where the T^{-2} dependence comes from the $T^{1/2}$ dependence of the thermal velocity and the $T^{3/2}$ dependence of the density of states and where we have assumed a temperature independent cross section. All other factors have been lumped into the

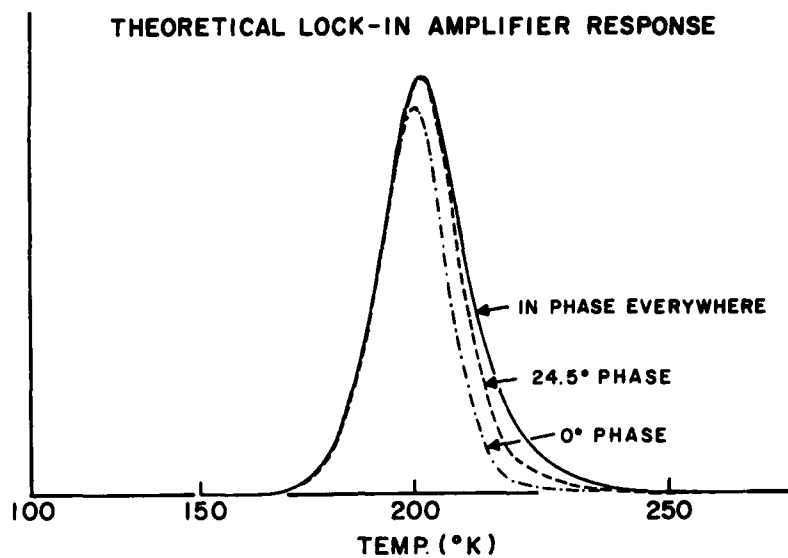


Figure 1. Theoretical Lineshapes for the Lock-In Amplifier Version of Capacitance Transient Spectroscopy for Different Lock-In Amplifier Phase Settings (Mixer 0° or 24.5° Before Beginning of Capacitance Transient) or for Phase Independent (Vector Amplitude) Output. The temperature scale is one appropriate for thermocouple output

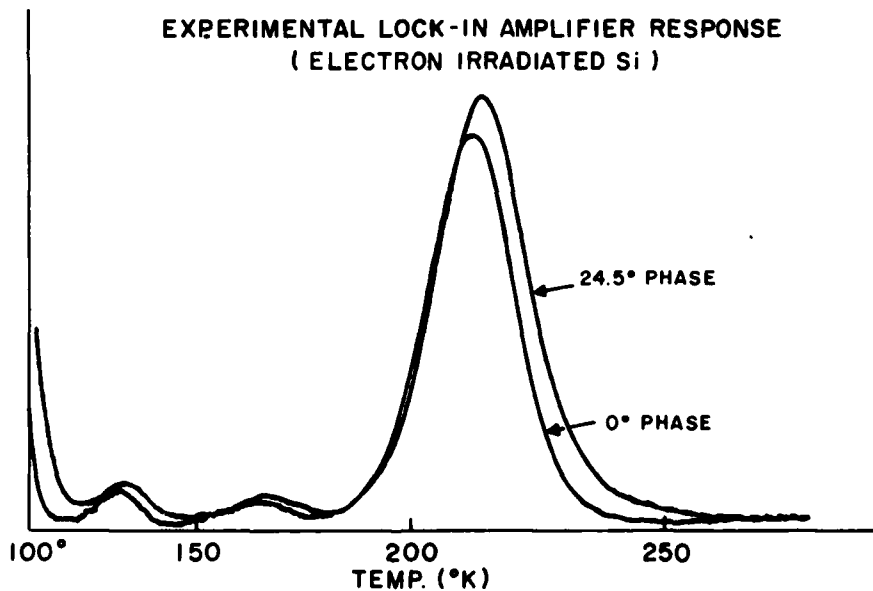


Figure 2. Experimental Spectra for the E-Center in Electron Irradiated Silicon for Two Lock-In Amplifier Phase Settings

constant C. We now choose two easily definable points on the lineshape curve $A(\alpha)$. For example, we might choose α_1 and α_2 such that $A(\alpha_1) = A(\alpha_2) = \frac{1}{2} A_{\max}$. From Eq. (20), there are two temperatures corresponding to the two α 's which equally well define these half-maximum points. If $\alpha_1 < \alpha_2$ and $T_1 < T_2$, then α_1 corresponds to T_2 and α_2 corresponds to T_1 , since large α means small T. We can thus write

$$\alpha_1 = C T_2^{-2} e^{\Delta E/kT_2} \quad (21)$$

and

$$\alpha_2 = C T_1^{-2} e^{\Delta E/kT_1} \quad (22)$$

Taking the natural logarithm of both equations, we get

$$\ln \alpha_1 = \ln C - 2 \ln T_2 + \frac{\Delta E}{kT_2} \quad (23)$$

$$\ln \alpha_2 = \ln C - 2 \ln T_1 + \frac{\Delta E}{kT_1} \quad (24)$$

Subtracting Eq. (23) from Eq. (24), we get

$$\ln \frac{\alpha_2}{\alpha_1} = \frac{\Delta E}{kT_1} - \frac{\Delta E}{kT_2} + 2 \ln \frac{T_2}{T_1} \quad (25)$$

or

$$\Delta E = \frac{k \ln \frac{\alpha_2}{\alpha_1}}{\frac{1}{T_1} - \frac{1}{T_2}} - 2k \left(\frac{\ln \frac{T_2}{T_1}}{\frac{1}{T_1} - \frac{1}{T_2}} \right) \quad (26)$$

If we use the approximation

$$\ln x \cong 2 \left(\frac{x-1}{x+1} \right) \quad (27)$$

for x not too far from unity, and if we write

$$T_2 = T_{av} + \Delta \quad (28)$$

$$T_1 = T_{av} - \Delta$$

where T_{av} is the average of T_1 and T_2 , we find

$$\left(\frac{\ln \frac{T_2}{T_1}}{\frac{1}{T_1} - \frac{1}{T_2}} \right) \cong T_{av} + \frac{\Delta^2}{T_{av}} \cong T_{av} \cong T_{max} \quad (29)$$

Equation (26) can then be written

$$\Delta E = \frac{k \ln \frac{\alpha_2}{\alpha_1}}{\frac{1}{T_1} - \frac{1}{T_2}} - 2kT_{max} \quad (30)$$

This result has been derived by others for the 0° phase lineshape.¹⁰ As mentioned above, one need not use the half-maximum points. If one only had half the curve, for example, the one-half maximum point and the full maximum point could be used. If the left half of the curve (from a temperature viewpoint) were available, one could get the activation energy from

$$\Delta E = \frac{k \ln \left(\frac{\alpha_2}{\alpha_{max}} \right)}{\frac{1}{T_1} - \frac{1}{T_{max}}} - 2kT_{max} \quad (31)$$

Errors due to noise in the experimentally determined lineshape are just compounded when the two points chosen are close together. It is advisable, therefore, to use the two half-maximum points.

In order to do all of this, the appropriate points on the experimental curves must be able to be accurately determined. This means that a good clean trace with an obvious baseline must be available. If there is a weak, noisy signal, or one whose baseline is not obvious, it is better to do an Arrhenius plot from a number of scans.

10. Kimerling, L.C., private communication.

Table 1 gives the parameters necessary to perform the above calculations for the various lock-in phase settings.

Table 1. Lineshape Expressions and Values of Parameters Defined in the Text, for Various Lock-In Amplifier Phase Settings

	0°	24.5°	Ph-ind.
$A(\alpha)$	$\frac{8\alpha^2(1-e^{-1/\alpha})}{4\pi^2\alpha^2+1}$	$\frac{4\alpha(1-e^{-1/\alpha})}{\pi(4\pi^2\alpha^2+1)^{1/2}} \cos(\tan^{-1} \frac{1}{2\pi\alpha} - \phi)$	$\frac{4\alpha(1-e^{-1/\alpha})}{\pi(4\pi^2\alpha^2+1)^{1/2}}$
α_{\max}	0.4243	0.3485	0.3485
A_{\max}	0.1608	0.1739	0.1739
$\frac{\text{sq. wave resp.}^*}{\text{exp. resp.}}$	2.52	2.33	2.33
α_1	0.1291	0.09657	0.07559
α_2	1.9613	1.643	1.775
$\frac{\alpha_2}{\alpha_1}$	15.19	17.01	23.48
$\frac{\alpha_2}{\alpha_{\max}} \dagger$	4.622	4.715	5.093
$\frac{\alpha_{\max}}{\alpha_1} \ddagger$	3.286	3.609	4.610

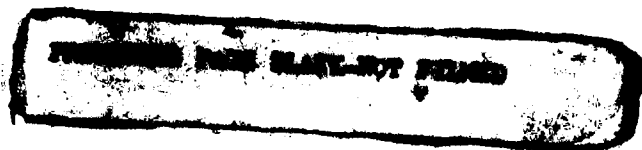
* Ratio of unit square wave response (phase set for maximum response) to unit exponential train response (phase set to indicated value).

† For calculating activation energy from left hand side of peak lineshape.

‡ For calculating activation energy from right hand side of peak lineshape.

References

1. Miller, G.L., Lang, D.V., and Kimerling, L.C. (1977) Ann. Rev. Mat. Sci. 1977:377.
2. Lang, D.V. (1974) J. Appl. Phys. 45:3023.
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9. Schott, J.T., DeAngelis, H.M., and White, W.R. (1976) Air Force Technical Report, AFCRL-TR-76-0024.
10. Kimerling, L.C. private communication.



Appendix

Computer Plotted Spectra

The following program plots capacitance transient spectra, given the input of activation energy, effective cross section and amplitude for each level. The comment statements at the beginning of the program describe it more fully. It is written in Tektest III language for use with a Tektronix S-3260 integrated circuit test system.

To run the program, ensure that the proper disc (A65B Hanscom) is in operation. Then, after typing:

ctrl C

to obtain the executive prompter (\$), type either:

DRIVE 0

or:

DRIVE 1

followed by a carriage return (CR), depending on which drive contains the proper disc. Then type:

IDENT SCH

followed by a CR, and then:

RUN DLTS

followed by a CR. You then enter data as requested by the computer.

DLTS.EDT: SCH
DATE 27-APR-79

TIME 10:14

DISK NAME: A65B HANSCOM
PAGE 1 OF 7

```
1.0100 *          TRANSIENT CAPACITANCE SPECTROSCOPY
1.0200 *          WRITTEN BY
1.0300 *          JOHN T. SCHOTT
1.0400 *          (LATEST REVISION-FEB 79)
1.0500 *
1.0600 * THIS PROGRAM PLOTS COMBINED AND INDIVIDUAL TRANSIENT CAPACITANCE
1.0700 * (DLTS) SPECTRA AND SUPERPOSITIONS OF THE TWO. IT ASSUMES THE
1.0800 * USE OF A LOCK-IN AMPLIFIER WITH VARIOUS PHASE SETTING OPTIONS.
1.0900 * MATERIAL CONSTANTS CAN BE SET FOR EITHER N- OR P-TYPE SILICON
1.1000 * OR GALLIUM ARSENIDE. TEMPERATURE IS PLOTTED ON A SCALE APPRO-
1.1100 * PRIATE FOR A COPPER-CONSTANTAN THERMOCOUPLE. HARD COPY
1.1200 * IMAGE SIZE MAY BE ADJUSTED TO DUPLICATE SCALE OF EXPERIMENTAL
1.1300 * TRACES BY APPROPRIATE TEMPERATURE RANGE INPUT AND ADJUSTMENT
1.1400 * OF 'SCALE' VALUES.

2.1000 SUBROUTINE DCOORD(4),SCCOORD(4):GRAPHU
2.2000 SUBROUTINE VECTR(4),CURSOR(2),DRAWU(3):GRAPHU
2.3000 ARRAY E(10),SIGMA(10),AMP(10)
2.4000 ARRAY X(4),Y(4),S2(4)
2.5000 ARRAY EI(10),SIGMAI(10),AMPI(10)
2.6000 ARRAY EC(10),SIGMAC(10),AMP(10)

3.0100 PRESET X=-252.87,-195.802,0,100
3.0200 PRESET Y=-6.197755,-5.535673,0,4.27961
3.0300 PRESET S2=.241816E-3,.1355393E-3,.9026148E-4,.720794E-4
3.0400 CONSTANT K=8.62E-5
3.0500 CONSTANT PHASE=.4284029
3.0600 CONSTANT PI=3.141593
3.0700 CONSTANT C1=2E-22
3.0800 CONSTANT C2=5E-22
3.0900 CONSTANT C3=5E-21
3.1000 CONSTANT C4=7E-22

4.0010 * ACCEPT INPUT INFORMATION
4.0020 AGAIN = 0
4.0030 PRINT CR
4.0040 PRINT 'LOCK-IN AMPLIFIER PHASE SETTINGS ARE CODED AS FOLLOWS:',CR
4.0050 PRINT '      1. IN PHASE WITH BIAS PULSE',CR
4.0060 PRINT '      2. 24.5 DEG BEFORE BIAS PULSE',CR
4.0070 PRINT '      3. PHASE INDEPENDENT (VECTOR AMP OUTPUT)',CR
4.0080 PRINT 'ENTER NUMBER FOR PHASE SETTING:'
4.0090 IF(AGAIN) 4.012
4.0100 ACCEPT PHAS
4.0110 GO TO 4.015
4.0120 ACCEPT CHANGE
4.0130 IF(CHANGE EQ 0) 4.019
4.0140 PHAS = CHANGE
4.0150 IF(PHAS NE INT(PHAS)) 4.017
4.0160 IF(1<PHAS<3) 4.019
4.0170 PRINT 'TRY AGAIN',CR
4.0180 GO TO 4.008
4.0190 PRINT 'MATERIAL TYPES ARE CODED AS FOLLOWS:',CR
4.0200 PRINT '      1. N-TYPE SILICON',CR
4.0210 PRINT '      2. P-TYPE SILICON',CR
4.0220 PRINT '      3. N-TYPE GALLIUM ARSENIDE',CR
4.0230 PRINT '      4. P-TYPE GALLIUM ARSENIDE',CR
4.0240 PRINT 'ENTER NUMBER FOR MATERIAL TYPE:'
```

DLTS.EDT:SCH
DATE 27-APR-79

TIME 10:14

DISK NAME: A65B HANSCOM
PAGE 2 OF 7

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4.0250 IF(AGAIN) 4.028
4.0260 ACCEPT MAT
4.0270 GO TO 4.031
4.0280 ACCEPT CHANGE
4.0290 IF(CHANGE EQ 0) 4.045
4.0300 MAT = CHANGE
4.0310 IF(MAT NE INT(MAT)) 4.033
4.0320 IF(1<MAT<4) 4.035
4.0330 PRINT 'TRY AGAIN',CR
4.0340 GO TO 4.024
4.0350 IF(MAT NE 1) 4.038
4.0360 C = C1
4.0370 GO TO 4.045
4.0380 IF(MAT NE 2) 4.041
4.0390 C = C2
4.0400 GO TO 4.045
4.0410 IF(MAT NE 3) 4.044
4.0420 C = C3
4.0430 GO TO 4.045
4.0440 C = C4
4.0450 PRINT 'DO YOU WANT POS. PEAKS (ENTER 1), NEG. PEAKS (ENTER -1), '
4.0460 PRINT CR, 'OR BOTH (ENTER 0)?; '
4.0470 IF(AGAIN) 4.05
4.0480 ACCEPT YRANGE
4.0490 GO TO 4.056
4.0500 ACCEPT CHANGE
4.0510 IF(CHANGE EQ 0) 4.056
4.0520 IF(CHANGE NE 999) 4.055
4.0530 YRANGE=0
4.0540 GO TO 4.056
4.0550 YRANGE=CHANGE
4.0560 PRINT 'ENTER TEMP RANGE IN DEG KELVIN (25<T<350)',CR
4.0570 IF(AGAIN) 4.06
4.0580 ACCEPT 'TMIN=',TMIN
4.0590 GO TO 4.063
4.0600 ACCEPT 'TMIN=',CHANGE
4.0610 IF(CHANGE EQ 0) 4.069
4.0620 TMIN=CHANGE
4.0630 IF(25<TMIN<350) 4.066
4.0640 PRINT 'TEMP OUT OF RANGE 25<T<350',CR
4.0650 GO TO 4.057
4.0660 IF(AGAIN) 4.069
4.0670 ACCEPT 'TMAX=',TMAX
4.0680 GO TO 4.072
4.0690 ACCEPT 'TMAX=',CHANGE
4.0700 IF(CHANGE EQ 0) 4.081
4.0710 TMAX=CHANGE
4.0720 IF(TMAX LE 350)4.075
4.0730 PRINT 'TEMP OUT OF RANGE 25<T<350',CR
4.0740 GO TO 4.066
4.0750 IF(TMAX GT TMIN) 4.078
4.0760 PRINT 'TRY AGAIN',CR
4.0770 GO TO 4.056
4.0780 IF(AGAIN) 4.081
4.0790 ACCEPT 'WHAT IS THE LOCK-IN FREQUENCY?; ',F
4.0800 GO TO 4.086
4.0810 ACCEPT 'WHAT IS THE LOCK-IN FREQUENCY?; ',CHANGE
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DLTS.EDT:SCH
DATE 27-APR-79

TIME 10:14

DISK NAME: A65B HANSCOM
PAGE 3 OF 7

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4.0820 IF(CHANGE EQ 0) 4.088
4.0830 F=CHANGE
4.0840 GO TO 4.088
4.0850 IF(AGAIN) 4.088
4.0860 ACCEPT 'HOW MANY PEAKS FOR THE COMBINED SPECTRUM?: ',N
4.0870 GO TO 4.094
4.0880 ACCEPT 'HOW MANY PEAKS FOR THE COMBINED SPECTRUM?: ',CHANGE
4.0890 IF(CHANGE EQ 0) 4.094
4.0900 IF(CHANGE NE 999) 4.093
4.0910 N=0
4.0920 GO TO 4.124
4.0930 N=CHANGE
4.0940 IF(1<N<10) 4.124,4.097,4.095
4.0950 PRINT 'THAT'S A BIT MUCH',CR
4.0960 GO TO 4.085
4.0970 LOOP 4.123 J=1,N
4.0980 PRINT CR
4.0990 PRINT 'ENTER ACTIVATION ENERGY IN EV FOR PEAK ',J:IOC,': '
4.1000 IF(AGAIN) 4.103
4.1010 ACCEPT EC(J)
4.1020 GO TO 4.106
4.1030 ACCEPT CHANGE
4.1040 IF(CHANGE EQ 0) 4.106
4.1050 EC(J)=CHANGE
4.1060 PRINT 'ENTER CROSS SECTION IN SQ CM FOR PEAK ',J:IOC,': '
4.1070 IF(AGAIN) 4.111
4.1080 ACCEPT SIGMAC(J)
4.1090 GO TO 4.113
4.1100 ACCEPT CHANGE
4.1110 IF(CHANGE EQ 0) 4.113
4.1120 SIGMAC(J)=CHANGE
4.1130 PRINT 'ENTER AMPLITUDE (POS. OR NEG.) IN CM FOR PEAK ',J:IOC,': '
4.1140 IF(AGAIN) 4.117
4.1150 ACCEPT AMPC(J)
4.1160 GO TO 4.123
4.1170 ACCEPT CHANGE
4.1180 IF(CHANGE EQ 0) 4.123
4.1190 IF(CHANGE NE 999) 4.122
4.1200 AMPC(J)=0
4.1210 GO TO 4.123
4.1220 AMPC(J)=CHANGE
4.1230 CONTINUE
4.1240 PRINT CR,'DO YOU WANT ANY PEAKS PLOTTED INDIVIDUALLY? ',CR
4.1250 IF (AGAIN) 4.128
4.1260 ACCEPT 'IF SO, ENTER THE NUMBER; OTHERWISE HIT CR: ',NI
4.1270 GO TO 4.134
4.1280 ACCEPT 'IF SO, ENTER THE NUMBER; OTHERWISE ENTER 999: ',CHANGE
4.1290 IF(CHANGE EQ 0) 4.134
4.1300 IF(CHANGE NE 999) 4.133
4.1310 NI=0
4.1320 GO TO 5.01
4.1330 NI=CHANGE
4.1340 IF(1<NI<10) 5.01,4.137,4.135
4.1350 PRINT 'THAT'S A BIT MUCH.',CR
4.1360 GO TO 4.125
4.1370 IF(N NE NI) 4.154
4.1380 PRINT CR
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DLTS.EDT: SCH
DATE 27-APR-79

TIME 10:14

DISK NAME: A65B HANSCOM
PAGE 4 OF 7

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4.1390 PRINT 'IF THESE ARE THE SAME PEAKS AS FOR THE COMBINED SPECTRUM, ', CR
4.1400 IF (AGAIN) 4.143
4.1410 ACCEPT 'ENTER +1; OTHERWISE, HIT CR: ', SAME
4.1420 GO TO 4.147
4.1430 ACCEPT 'ENTER +1; OTHERWISE, ENTER 999: ', CHANGE
4.1440 IF (CHANGE EQ 0) 4.147
4.1450 IF (CHANGE EQ 999) 4.155
4.1460 SAME=CHANGE
4.1470 IF (SAME EQ 0) 4.155
4.1480 LOOP 4.152 J=1, N
4.1490 EI(J)=EC(J)
4.1500 SIGMAI(J)=SIGMAC(J)
4.1510 AMPI(J)=AMPC(J)
4.1520 CONTINUE
4.1530 GO TO 5.01
4.1540 SAME=0
4.1550 LOOP 4.181 J=1, NI
4.1560 PRINT CR
4.1570 PRINT 'ENTER ACTIVATION ENERGY IN EV FOR PEAK I-', J:IOC, ': '
4.1580 IF (AGAIN) 4.161
4.1590 ACCEPT EI(J)
4.1600 GO TO 4.164
4.1610 ACCEPT CHANGE
4.1620 IF (CHANGE EQ 0) 4.164
4.1630 EI(J)=CHANGE
4.1640 PRINT 'ENTER CROSS SECTION IN SQ CM FOR PEAK I-', J:IOC, ': '
4.1650 IF (AGAIN) 4.168
4.1660 ACCEPT SIGMAI(J)
4.1670 GO TO 4.171
4.1680 ACCEPT CHANGE
4.1690 IF (CHANGE EQ 0) 4.171
4.1700 SIGMAI(J)=CHANGE
4.1710 PRINT 'ENTER AMPLITUDE (POS. OR NEG.) IN CM FOR PEAK I-', J:IOC, ': '
4.1720 IF (AGAIN) 4.175
4.1730 ACCEPT AMPI(J)
4.1740 GO TO 4.181
4.1750 ACCEPT CHANGE
4.1760 IF (CHANGE EQ 0) 4.181
4.1770 IF (CHANGE NE 999) 4.18
4.1780 AMPI(J)=0
4.1790 GO TO 4.181
4.1800 AMPI(J)=CHANGE
4.1810 CONTINUE

5.0100 * DRAW AXES
5.0200 PRINT ERASE
5.0300 VECTRF (40, 780, 40, 110)
5.0400 VECTRF (7, 700, 12, 716)
5.0500 VECTRF (12, 716, 17, 700)
5.0600 VECTRF (17, 700, 7, 700)
5.0700 CURSOR (21, 700)
5.0800 PRINT 'C'
5.0900 VECTRF (40, 110, 1000, 110)
5.1000 VECTRF (1000, 110, 1000, 780)
5.1100 VECTRF (1000, 780, 40, 780)
5.1200 CURSOR (967, 66)
5.1300 PRINT 'TEMP'
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DLTS.EDT:SCH

DISK NAME: A65B HANSCOM

DATE 27-APR-79

TIME 10:14

PAGE 5 OF 7

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6.0100 * DRAW SCALE ON HORIZONTAL AXIS
6.0200 TMIN=INT(TMIN)
6.0300 TMAX=INT(TMAX)
6.0400 TK=TMAX
6.0500 CALL 9.01
6.0600 EMFMAX=EMF
6.0700 TK=TMIN
6.0800 CALL 9.01
6.0900 EMFMIN=EMF
6.1000 SCALE=(EMFMAX-EMFMIN)/70
6.1100 DCOORD(EMFMIN-1.5*SCALE,EMFMAX,-22,4)
6.1200 SCOORD(19,1000,88,114)
6.1300 LOOP 6.21 TK=TMIN,TMAX
6.1400 IF(TK/50 NE INT(TK/50))6.2
6.1500 CALL 9.01
6.1600 DRAWV(EMF,4,0)
6.1700 DRAWV(EMF,-4,1)
6.1800 DRAWV(EMF-1.5*SCALE,-22,-1)
6.1900 PRINT TK:IOC
6.2000 CONTINUE
6.2100 CONTINUE
6.2200 DRAWV(EMFMIN,0,0)

7.0100 * CALCULATE AND DRAW DLTS SPECTRA
7.0200 * ('SCALE' VALUES MUST BE ADJUSTED FOR HARD COPY IMAGE SIZE)
7.0300 IF(PHASE 1) 7.06
7.0400 SCALE = 2.31
7.0500 GO TO 7.07
7.0600 SCALE = 2.48
7.0700 SCOORD(40,1000,110,780)
7.0800 IF(YRANGE) 7.09,7.11,7.14
7.0900 DCOORD(EMFMIN,EMFMAX,-SCALE,0)
7.1000 GO TO 7.15
7.1100 DCOORD(EMFMIN,EMFMAX,-SCALE/2,SCALE/2)
7.1200 VECTRF(40,445,1000,445)
7.1300 GO TO 7.15
7.1400 DCOORD(EMFMIN,EMFMAX,0,SCALE)
7.1500 IF(N LT 1) 7.31
7.1600 * -COMBINED SPECTRUM
7.1700 LOOP 7.21 J=1,N
7.1800 E(J)=EC(J)
7.1900 SIGMA(J)=SIGMAC(J)
7.2000 AMP(J)=AMPC(J)
7.2100 CONTINUE
7.2200 LOOP 7.3 TK=TMIN,TMAX,.5
7.2300 ASUM=0
7.2400 LOOP 7.27 J=1,N
7.2500 CALL 10.01
7.2600 ASUM = ASUM+A
7.2700 CONTINUE
7.2800 CALL 9.01
7.2900 DRAWV(EMF,ASUM,1)
7.3000 CONTINUE
7.3100 IF(NI LT 1) 8.01
7.3200 * -INDIVIDUAL SPECTRA
7.3300 LOOP 7.37 J=1,NI
7.3400 E(J)=E1(J)
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DLTS.EDT:SCH
DATE 27-APR-79

TIME 10:14

DISK NAME: A65B HANSCDM
PAGE 6 OF 7

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7.3500 SIGMA(J)=SIGMAI(J)
7.3600 AMP(J)=AMPI(J)
7.3700 CONTINUE
7.3800 LOOP 7.49 J=1,NI
7.3900 DRAWV(EMFMIN,0,0)
7.4000 LOOP 7.48 TK=THIN,TMAX,.5
7.4100 CALL 10.01
7.4200 CALL 9.01
7.4300 IF(TK EQ INT(TK)) 7.46
7.4400 DRAWV(EMF,A,1)
7.4500 GO TO 7.47
7.4600 DRAWV(EMF,A,0)
7.4700 CONTINUE
7.4800 CONTINUE
7.4900 CONTINUE
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8.0100 * PRINT INPUT INFO
8.0200 CURSOR(770,44)
8.0300 IF(MAT NE 1) 8.06
8.0400 PRINT "N-SI"
8.0500 GO TO 8.13
8.0600 IF(MAT NE 2) 8.09
8.0700 PRINT "P-SI"
8.0800 GO TO 8.13
8.0900 IF(MAT NE 3) 8.12
8.1000 PRINT "N-GAAS"
8.1100 GO TO 8.13
8.1200 PRINT "P-GAAS"
8.1300 IF(PHAS NE 1) 8.16
8.1400 PRINT " (0 DEG)"
8.1500 GO TO 8.2
8.1600 IF(PHAS NE 2) 8.19
8.1700 PRINT " (24.5 DEG)"
8.1800 GO TO 8.2
8.1900 PRINT " (PH IND)"
8.2000 CURSOR(714,22)
8.2100 PRINT F:R1,"HZ"
8.2200 CURSOR(742,0)
8.2300 PRINT TMIN:I0,"< T < ",TMAX:I0C
8.2400 CURSOR(0,44)
8.2500 IF(N EQ 0) 8.3
8.2600 LOOP 8.29 J=1,N
8.2700 PRINT "PEAK ",J:I0C,";"H",EC(J):R3C," EV; ",SIGMAC(J):E2C
8.2800 PRINT " SQ CM; AMPL=",AMPC(J):F3C,"CM",CR
8.2900 CONTINUE
8.3000 IF(NI EQ 0) 8.36
8.3100 IF(SAME EQ 1) 8.36
8.3200 LOOP 8.35 J=1,NI
8.3300 PRINT "PEAK I-",J:I0C,";"H",EI(J):R3C," EV; ",SIGMAI(J):E2C
8.3400 PRINT " SQ CM; AMPL=",AMPI(J):F3C,"CM",CR
8.3500 CONTINUE
8.3600 PRINT CR,CR
8.3700 GO TO 11.01
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```
9.0100 * CALCULATION OF APPROXIMATE!! EMF AS FUNCTION OF T
9.0200 * (SEE "TEMPERATURE, ITS MEAS & CTRL IN SCI & IND," VOL 4, PT 3,
9.0300 * ED. H.H.PLUMB (PITTSBURG,1972), PG. 1613.)
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DLTS.EDT:SCH

DATE 27-APR-79 TIME 10:14

DISK NAME: A65B HANSCOM

PAGE 7 OF 7

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9.0400 TC=TK-273
9.0500 I=2
9.0600 IF(TC LT X(3))9.09
9.0700 I=3
9.0800 GO TO 9.13
9.0900 IF(TC-X(I)) 9.12,9.13,9.1
9.1000 I=I+1
9.1100 GO TO 9.09
9.1200 I=I-1
9.1300 HT1=TC-X(I)
9.1400 HT2=TC-X(I+1)
9.1500 PROD=HT1*HT2
9.1600 H=X(I+1)-X(I)
9.1700 DELY=(Y(I+1)-Y(I))/H
9.1800 S3=(S2(I+1)-S2(I))/H
9.1900 SS2=S2(I)+HT1*S3
9.2000 DELSQS=(S2(I)+S2(I+1)+SS2)/6
9.2100 EMF=Y(I)+HT1*DELY+PROD*DELSQS
9.2200 RETURN

10.0100 * CALCULATION OF DLTS CURVE AMPLITUDE
10.0200 * ('IF' STATEMENTS AVOID EXCEEDING RANGE OF 10**-38 TO 10**+38)
10.0300 IF(E(J)/(K*TK) LT 86) 10.06
10.0400 A=0
10.0500 GO TO 10.17
10.0600 POWR1=EXP(E(J)/(K*TK))
10.0700 ALPHA=F*K*POWR1/(SIGMA(J)*TK**2)
10.0800 IF(ALPHA GT .013) 10.11
10.0900 POWR2=0
10.1000 GO TO 10.15
10.1100 POWR2=EXP(-1/ALPHA)
10.1200 IF(E(J)/(K*TK) LT 43) 10.15
10.1300 A1=AMP(J)**2*(1-POWR2)/PI**2
10.1400 GO TO 10.19
10.1500 IF(PHASE NE 1) 10.18
10.1600 A = AMP(J)**8*ALPHA**2*(1-POWR2)/(4*PI**2*ALPHA**2+1)
10.1700 GO TO 10.23
10.1800 A1 = AMP(J)**4*ALPHA*(1-POWR2)/(PI*SQRT(4*PI**2*ALPHA**2+1))
10.1900 IF(PHASE NE 2) 10.22
10.2000 A = A1*COS(ATAN(1/(2*PI*ALPHA)))-PHASE
10.2100 GO TO 10.23
10.2200 A = A1
10.2300 RETURN

11.0100 * ALLOW REPEAT WITH SOME INPUT INFO CHANGED
11.0200 PRINT 'IF YOU WANT A REPEAT WITH SOME INPUT DATA CHANGED,',CR
11.0300 ACCEPT 'HIT CR; OTHERWISE ENTER 1:', REPT
11.0400 IF(REPT NE 0) 11.11
11.0500 PRINT CR,'AS INPUT DATA IS REQUESTED, IF YOU WISH THAT QUANTITY',CR
11.0600 PRINT 'UNCHANGED, SIMPLY HIT CR.',CR
11.0700 PRINT '(NOTE: TO CHANGE A NON-ZERO VALUE TO ZERO, YOU MUST',CR
11.0800 PRINT 'ENTER 999.)',CR
11.0900 AGAIN=REPT+1
11.1000 GO TO 4.003
11.1100 STOP
```