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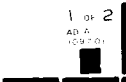

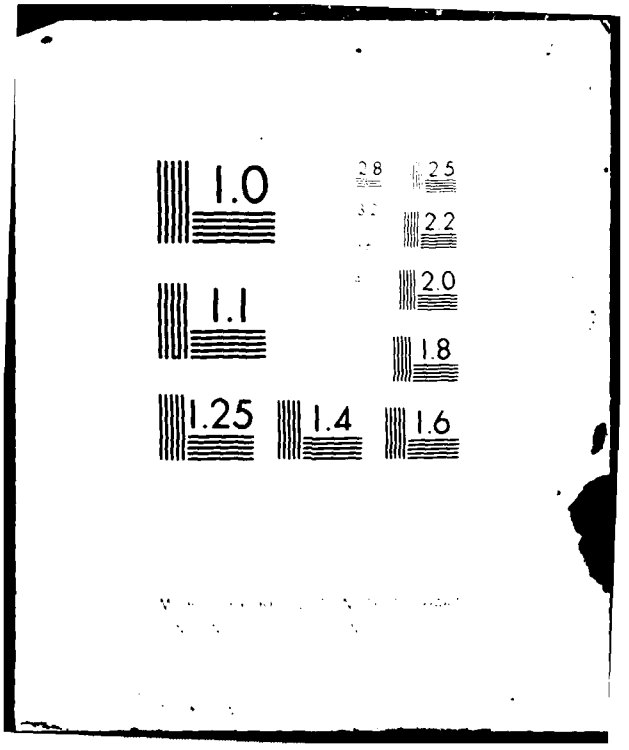
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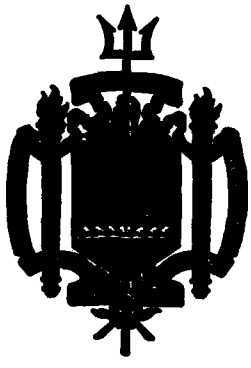

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1981

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a very powerful experimental method using the transient capacitance properties reverse-biased p-n junction diodes to characterize defects. A particular electron trap in n-type GaAlAs, known as the DX center is studied in this report using two different DLTS experimental setups. A complex model is proposed for the DX center consisting of a group plus an excited state with independent capture cross sections and communication between the two levels. Since classical analysis of DLTS data yields misleading results when a complex trap is considered, a computer simulation and curve fitting technique was used to determine the trap structure and parameters. This technique gave values of .295 eV for the ground state energy, .219 eV for the excited state, prefactor values on the ground, excited, and communication prefactor of 1.02×10^7, 2.2×10^8, and 5.58×10^5, respectively.

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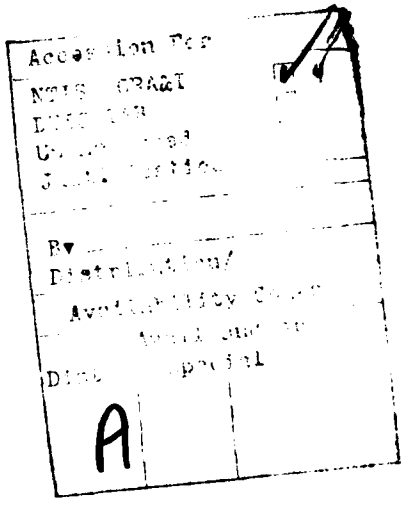

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"Characterization of Trapping States in Semiconductors"

A Trident Scholar Project Report

by

Midshipman Harvey S. Hopkins, Class of 1981
U. S. Naval Academy
Annapolis, Maryland

Robert N. Shelby

Advisor: Prof. Robert N. Shelby
Physics Department

Accepted for Trident Scholar Committee

Chairman

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Date

ABSTRACT

Defect energy states within the band gap are known to affect the performance of semiconductors in terms of response time. The characterization of defects is the first step in understanding how they act and how one may use them to benefit diode performance. Characterization of a defect includes among other quantities, the energy difference from the band edge, and the capture cross section of the energy state. Deep Level Transient Spectroscopy (DLTS) is a very powerful experimental method using the transient capacitance properties reverse-biased p-n junction diodes to characterize defects. A particular electron trap in n-type GaAℓAs, known as the DX center is studied in this report using two different DLTS experimental setups. A complex model is proposed for the DX center consisting of a ground plus an excited state with independent capture cross sections and communication between the two levels. Since classical analysis of DLTS data yields misleading results when a complex trap is considered, a computer simulation and curve fitting technique was used to determine the trap structure and parameters. This technique gave values of .295 eV for the ground state energy, .219 eV for the excited state, prefactor values on the ground, excited, and communication prefactor of 1.02×10^{7}, 2.2×10^{8}, and 5.58×10^{5}, respectively.

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I would like to thank the people whose names do not appear on this report but were very helpful with my study. In the way of technical support, Mr. Richard Krebs and Mr. Hobert Smith were always ready to help with advice or assistance on the DLTS equipment. Mr. Fred Wasem oversaw the ordering of equipment and supplies for my apparatus.

The man responsible for tutoring me on the subtleties of APL was Professor Charles Rector. His modification of the curve fitting program to my use was instrumental in the later phases of the data analysis. Dr. Richard Magno contributed greatly by supplying data to me and also by allowing me to use his DLTS setup at the Naval Research Laboratory to take advantage of the increased sophistication of his techniques.

None of this work would have been possible without the support of my advisor, Professor Robert N. Shelby, who constantly guided my efforts on the computer and saved me countless hours of work when I was on the wrong track. Many times Professor Shelby came to my rescue when the DLTS apparatus was acting up. He supported me with guidance and confidence through any failures, and celebrated with me every success. For this, I am truly grateful.

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Chapter I

Introduction

The advent of the semiconductor as a useful electronic component has revolutionized the electronics field. The physical and electronic properties of a semiconductor can be controlled by doping to produce the properties desired by the design engineer. Studies of the doping centers have been numerous and complete as the knowledge of the energy levels and electron capture cross sections of dopants is essential to their application to produce a required effect. Manufacturing of semiconductor material introduces substitutional impurities or vacancies into the lattice which produce increased strain in the lattice, thus creating energy levels in the band gap which may trap electrons during transitions. Exposure to radiation or energetic implantation of dopants can also cause these electronic defects.

A useful method for measuring the energy of trapping states is Deep Level Transient Spectroscopy (DLTS) developed by D. V. Lang in 1974.[1] This method uses the transient capacitance properties of reverse-biased p-n junction diodes to measure the important trapping state parameters: trap energy, electron capture cross section, and trap concentration. DLTS produces data peaks based on a trap's characteristic emission rate. A classical type of analysis based on simple, one level energy states yields correct values for trap parameters when the sample contains

one level traps. When the energy levels are complex, the classical analysis yields convincing, but misleading, results as to the nature of the trap. A closer look at the data for a particular defect in GaAℓAs called the DX center, reveals that this defect may not be a simple single state trap, but can possibly be more accurately characterized by a ground-excited state model. Computer simulation of the DLTS response to various trap models supports this conclusion. The formulation and collection of data supporting the ground-excited state model comprised the bulk of this study. The DX center is responsible for changing the response time of the diode after a bias pulse, which is a critical factor in many high speed device applications, which makes its characterization a matter of great interest.

In Chapter II, basic semiconductor theory, doping, and defects are reviewed. Chapter III relates specific information on the DX center and diode samples used in this study. The experimental theory of DLTS is discussed in Chapter IV; the analysis and results of the data obtained as well as the trap model are presented in Chapter V. Chapter VI summarizes the major points and results of the experimental phase plus the model introduced.

Chapter II

Semiconductor Theory

II-1. Pure Semiconductors and Doping

A semiconductor material may not be defined within rigid requirements but exists as somewhat of a transition between a metal and an insulator. Primarily a material is classified on the basis of the size of its band gap and the position of its Fermi energy. As shown in Figure II-1(a), a metal's Fermi energy lies above the edge of the conduction band allowing the conduction electrons to move freely. A semiconductor's Fermi level lies within the energy gap between the valence and conduction bands. This gap may range from 1 to 3 eV in depth. An insulator is similar as shown but has a band gap depth ranging from 5 to 10 eV.

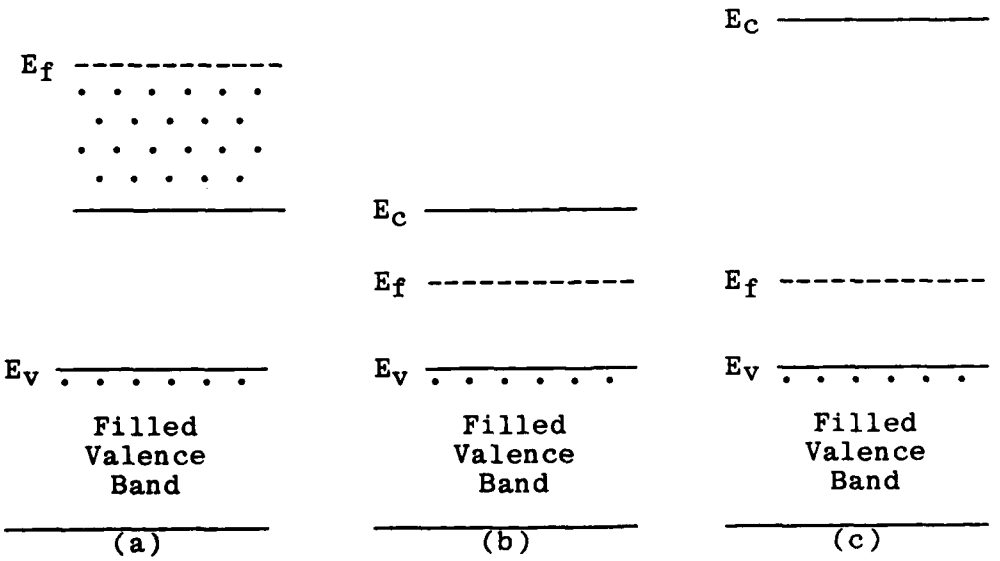


Figure II-1. Energy Levels for (a) a metal; (b) a semiconductor; and (c) an insulator.

As seen from the band gap diagrams, a semiconductor may conduct electricity if sufficient energy is given to electrons in the valence band to promote them to the conduction band. A pure semiconductor then acts as a temperature dependent resistor. To control a semiconductor's properties, impurity atoms are added to the host material. These dopants usually come from the III or V column of the Periodic Table and have energies close to the band gap edge. When ionized, these dopants release either majority or minority carriers depending on whether the impurity atom is a donor or acceptor and whether the material is doped as n or p type. An excess of acceptors creates p type material while an excess of donors creates n type material. The control of the spatial concentration of these dopants make it possible to make a device with the desired characteristics.

II-2. Semiconductor Defect States

Fundamentally, a defect or trap is an electron energy state in the band gap of a semiconductor as a result of the perturbation of the bonding structure of the host material by the presence of an impurity or lattice defect.[2] These defects may be classified as either shallow or deep states. Shallow states are related to defects in which an impurity atom is substituted at a lattice site for a host atom. The impurities are generally atoms which have a single excess (donor) or deficient (acceptor) valence

electron structure relative to the replaced atom. This type of state's descriptive name comes from its relative closeness to the edge of the band gap; conduction band for donors and valence band for acceptors. Shallow states in the past have been most easily studied using the technique of luminescence.[3]

Deep states are simply classified as defects whose energies place them deeper within the band gap. These states can be nonradiative recombination centers and as a result are not always receptive to investigation through luminescence.[4] DLTS though, as a transient capacitance technique yields much more information on deep states. Crystalline lattice defects as well as some dopants may cause deep states. Although the control of dopant concentration is well understood, there still exists some problems with impurity control in manufacturing processes. Also the effect of radiation damage, i.e., lattice defects, is not well understood as these crystalline defects can migrate through the lattice thereby changing defect concentration and the properties of the semiconductor itself at random.

Chapter III

The DX Center in GaAℓAs

The semiconductor investigated in this study is classified in the broad category of III-V compounds meaning that the constituent atoms come from the third and fifth columns of the periodic table. The III-V semiconductor is of great interest for its use in devices operating in the microwave frequency range as well as semiconductor lasers and light-emitting diodes.[5] Gallium Arsenide (GaAs) is the most popular of this new generation of semiconductors. Gallium Aluminum Arsenide (GaAℓAs), the variation of GaAs used in this study, is very similar to GaAs but with the advantage that the band gap can be varied over a small range by changing the relative aluminum concentration.

Each sample of GaAℓAs used has a seven-to-three ratio of gallium to aluminum. This mixture is expressed by writing $Ga_{.7}Al_{.3}As$ where three-tenths of the gallium atoms in the lattice have been replaced by aluminum atoms. Replacement by aluminum of the gallium is believed to cause changes in the annealing properties of the material which is of extreme importance to solid state device fabrication.[6] Defect stability is also enhanced by a two atom basis which makes migration through the lattice more difficult since a jump of two lattice spacings must be made instead of only one as in silicon semiconductors. The particular defect studied here is known as the "DX Center." Very little is

known about this defect except that it has been proposed to be made up of a donor impurity and a gallium vacancy.[7] The combination of a substitutional impurity with a vacancy creates much more lattice strain per defect than a substitution by itself. On the basis of radiation-induced length-change measurements and optical measurements in III-V compounds the lattice relaxation effects have been shown to be very strong.[8] This has a profound influence on the behavior of the DX center to act as a nonradiative recombination center. Irradiation of semiconductor laser materials with neutrons and, to a lesser degree, electrons has been shown to create DX centers in such concentration as to seriously degrade the operation of a laser in a very short time.[9] The employment of solid state devices in such hostile environments as outer space has created much interest in the study of these defects.

The samples used in this study are referred to by their laboratory number codes. The diode, L-107-C1A,1, is a beryllium implanted GaAℓAs p^+-n junction diode while S-214-BA1 and S-214-BB1 are Schottky barrier diodes. Both types of diodes react to DLTS in the same manner with but minor differences not affecting the experimental technique and analysis.

Chapter IV

Experimental Theory

IV-1. Mechanics of Carrier Capture and Emission

In a reverse-biased diode the traps within the depletion region are essentially empty of electrons. The method of DLTS relies on the ability to observe the emission of carriers from these traps so at some point they must be filled. This is done in the present case of a p^+-n junction by a majority carrier injection pulse. The diode is pulsed to zero bias, shoving the edge of the depletion region closer to the junction carrying with it electrons which are captured by the traps. At the end of the voltage pulse the depletion region again expands and as a result of the trapped electrons comes to rest beyond its quiescent reverse-biased equilibrium position. The capacitance of the diode changes radically with each phase of this process and will be discussed in detail in the next section. A transient phase of the process now takes place as the trapped electrons are thermally emitted back to the conduction band with the accompanying decrease in depletion region width for the case of the majority carrier injection pulse. See Figure IV-2.

The electron transitions to and from the conduction band are governed under equilibrium by the Principle of Detailed Balance which states that every transition is

balanced by its inverse. The system pictured is at equilibrium with the electron capture rate r_1 equal to the emission rate r_2.

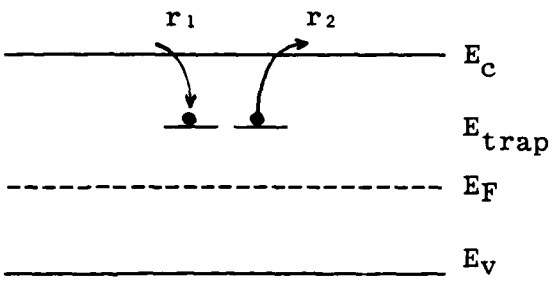


Figure IV-1. Principle of Detailed Balance

By applying this principle, the emission rate of a group of traps can be determined using Fermi-Dirac statistics. The capture rate is proportional to the number of empty traps, the number of electrons in the conduction band, the capture cross section of the trap, and the electron thermal velocity. The emission rate is proportional to the number of filled traps and the rate at which a single trap emits. The population of the traps may be found by multiplying their Fermi Function times the trap concentration. Some important parameters are:

σ	capture cross section
v	thermal velocity
n	number of electrons in the Conduction Band
N_t	total number of trapping states
f(E)	Fermi Function
e	trap emission rate

where $$f(E_t) = \frac{1}{e^{(E_t-E_F)/KT} + 1}$$

The capture and emission rates are given by:

$$r_1 = \sigma v n [1 - f(E_t)] N_t \qquad \text{(IV-1a)}$$

$$r_2 = N_t e f(E_t) \qquad \text{(IV-1b)}$$

At equilibrium these two rates are equal.

$$\sigma v n [1 - f(E_t)] N_t = N_t e f(E_t)$$

therefore

$$e = \sigma v n \frac{1 - f(E_t)}{f(E_t)} \qquad \text{(IV-1c)}$$

substituting in the Fermi Function

$$e = \sigma v n e^{(E_t-E_F)/KT} \qquad \text{(IV-1d)}$$

The number of electrons in the conduction band can be found using the effective density of states N_c times the Maxwell Boltzman Distribution which approximates the Fermi Function when $(E_c - E_F) >>> KT$.

$$n = N_c e^{(E_F-E_c)/KT} \qquad \text{(IV-1e)}$$

The density of states in the conduction band and the thermal velocity of the electrons is given below where m* is the effective mass of the electron.

$$N_c = 2\left[\frac{2m^*KT}{\hbar^2}\right]^{3/2} \qquad v = \left[\frac{3KT}{m^*}\right]^{1/2} \qquad \text{(IV-1f)}$$

Substituting all of this into the emission rate equation (IV-1d) gives

$$e = AT^2 e^{-\Delta E/KT} \qquad \text{(IV-1g)}$$

where $\Delta E = (E_c - E_t)$ $\qquad A = 4\sqrt{6}\,\frac{m^*K^2N_c}{\hbar^3}\,\sigma$

This is the rate at which an electron will be emitted from a single trap at depth ΔE and temperature T. This process determines the transient response of a diode which will play an important role in the proper operation of just about any solid state device.

IV-2. Transient Capacitance

The technique of DLTS uses the capacitance properties of a reverse-biased p-n junction to measure trap parameters. In keeping with this fact, it is necessary to know something about the properties of p-n junctions in the absence of traps. The simplest case is one of a p^+-n or n^+-p junction in uniformly doped material, with the + notation denoting the material being more heavily doped on the p or n side, respectively. This allows the depletion region to form almost entirely in the more lightly doped material simplifying the analysis greatly. The width W of the depletion region is given by:

$$W = \sqrt{\frac{2\varepsilon(V_{bi} + V)}{qN}} \qquad \text{(IV-2a)}$$

where ε is the dielectric constant of the depleted region, V_{bi} is the built-in bias of the junction, V is the applied reverse bias voltage, q is the electron charge, and N is the density of ionized doping centers in the lightly doped material. The same equation holds for Schottky barrier devices in which a metal coating is deposited on semiconductor material. The charge on the metal-semiconductor

interface must be taken into account, though, when calculating V_{bi}. A p^+-n junction thus acts like a voltage variable parallel plate capacitor with a layer of dielectric of constant ε and width W between electrodes. The width cannot be increased indefinitely though since one of three breakdown mechanisms will take over.

A depletion region devoid of free carriers is created when a reverse bias is applied since the electric field removes all free carriers. The edge of the region is where the electric field is zero, the applied bias being just balanced by all of the exposed ionized doping centers in the depletion region. In n type material the exposed centers are positive. Because of this effective area A of dielectric constant ε, the junction capacitance is simply given by:

$$C = \frac{\varepsilon A}{W} \qquad \text{(IV-2b)}$$

which is the same relationship for a parallel plate capacitor.

The addition of electron trapping states in the depletion region by doping, irradiating the sample causing lattice defects, or by unwanted impurities does not change Equation IV-2b. When these traps are filled as seen in Figure IV-2c the net effect is to decrease the junction capacitance by increasing the depletion region width.

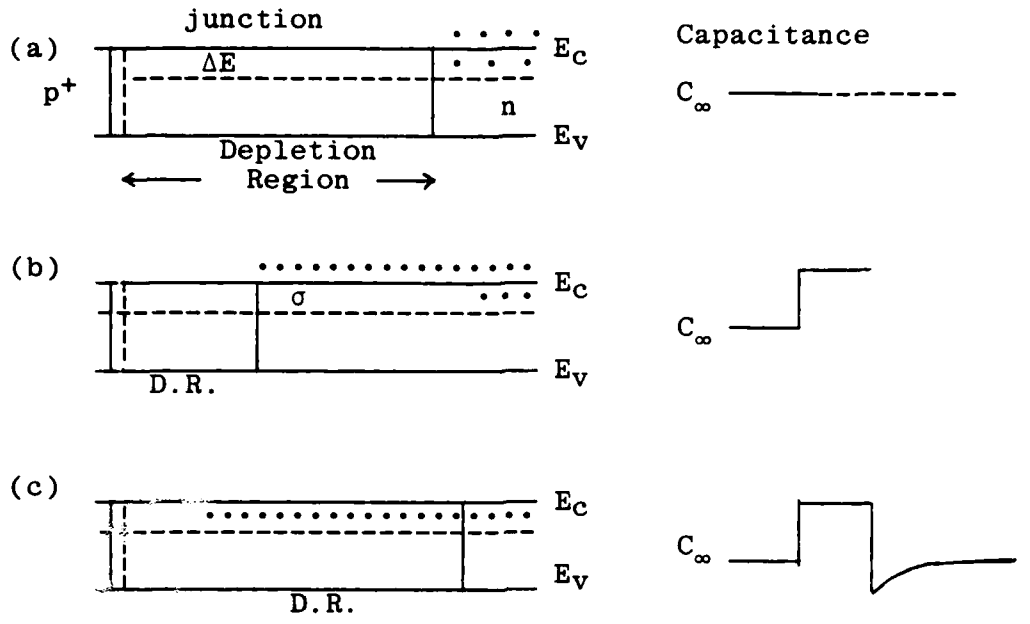


Figure IV-2. (a) Quiescent reverse bias situation and steady state capacitance; (b) majority carrier injection pulse; (c) trap emission phase with capacitance transient.

The relative capacitance change for n(x) trapped electrons within the depletion region in the interval Δx at x is given by:

$$\left[\frac{\Delta c}{c}\right]_x = - \left[\frac{n(x)}{N_+ W^2}\right] \times \Delta x \qquad \text{(IV-2c)}$$

where N_+ is the positive space charge concentration at W. Integrating over the entire depletion region gives the total change in capacitance where n(x) and N_+ are assumed constant.

$$\left[\frac{\Delta c}{c}\right]_{TOTAL} = - \tfrac{1}{2} \frac{n(x)}{N_+} \qquad \text{(IV-2d)}$$

The equation giving the actual change in capacitance with respect to electron emission rate and time can be derived starting with the following definition of the depletion width.

$$W = \sqrt{\frac{2\varepsilon V_{TOT}}{q}} \cdot \sqrt{\frac{1}{N_{DO} - N_{TO} e^{-et}}} \qquad \text{(IV-2e)}$$

where

q = electron charge

N_{DO} = total number of ionized donor sites

N_{TO} = total number of traps filled at $t = 0$

e = electron emission rate

$V_{TOT} = V_{bi} + V$

N_{DO} appears since in n type material $N_D >> N_a$ where N_a is the number of acceptor sites. The capacitance per unit area is then given by:

$$C(t) = \frac{\varepsilon}{W} = \sqrt{\frac{q\varepsilon N_{DO}}{2V_{TOT}}} \left[1 - \frac{N_{TO}}{N_{DO}} e^{-et}\right]^{\frac{1}{2}} \qquad \text{(IV-2f)}$$

With $N_{DO} >> N_{TO}$ this can be approximated by:

$$C(t) = \sqrt{\frac{q\varepsilon N_{DO}}{2V_{TOT}}} \left[1 - \frac{1}{2} \frac{N_{TO}}{N_{DO}} e^{-et}\right] \qquad \text{(IV-2g)}$$

The quantity actually measured in the DLTS experiment is the change in capacitance from the steady state value C_∞.

$$\Delta C(t) = C(t) - C_\infty = -C_\infty \frac{N_{TO}}{2N_{DO}} e^{-et} \qquad \text{(IV-2h)}$$

Thus the equilibrium reverse biased capacitance is given by:

$$C_\infty = \sqrt{\frac{q\varepsilon N_{DO}}{2V_{TOT}}} \qquad \text{(IV-2i)}$$

while the capacitance directly following the injection pulse before emission starts is half the steady state value. Quantities are defined in Figure IV-3.

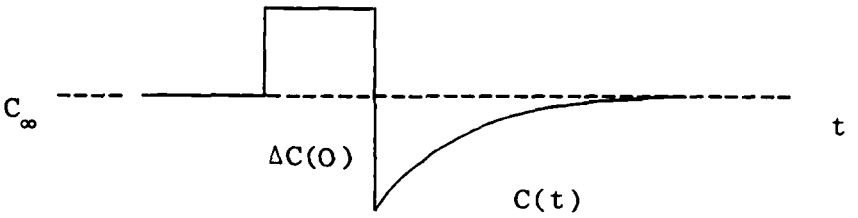


Figure IV-3. Capacitance Response to Majority Carrier Pulse

The response of a p^+-n junction discussed in this section is crucial to the DLTS method. The preceding treatment assumes uniform doping in the depletion region. Non-uniform doping yields a more complicated movement of the outer edge of the depletion region with bias pulses. All samples used in the DLTS runs were of uniform doping and do conform to the discussion presented. An explanation on the operation of the DLTS systems will now be presented.

IV-3. DLTS Experimental Apparatus

Two Deep Level Transient Spectroscopy experimental setups were used to obtain data. Both setups are very

similar and basically differ only in the components used to analyze the capacitive transient and produce the familiar DLTS peak.

The first DLTS setup utilizing a double boxcar integrator for signal processing and output is located at the Naval Research Laboratory in Washington, D. C. This system built by Dr. Richard Magno was used to obtain the data actually used to test the ground-excited state model of the DX center in GaAℓAs. A schematic of this system is shown in Figure IV-4.

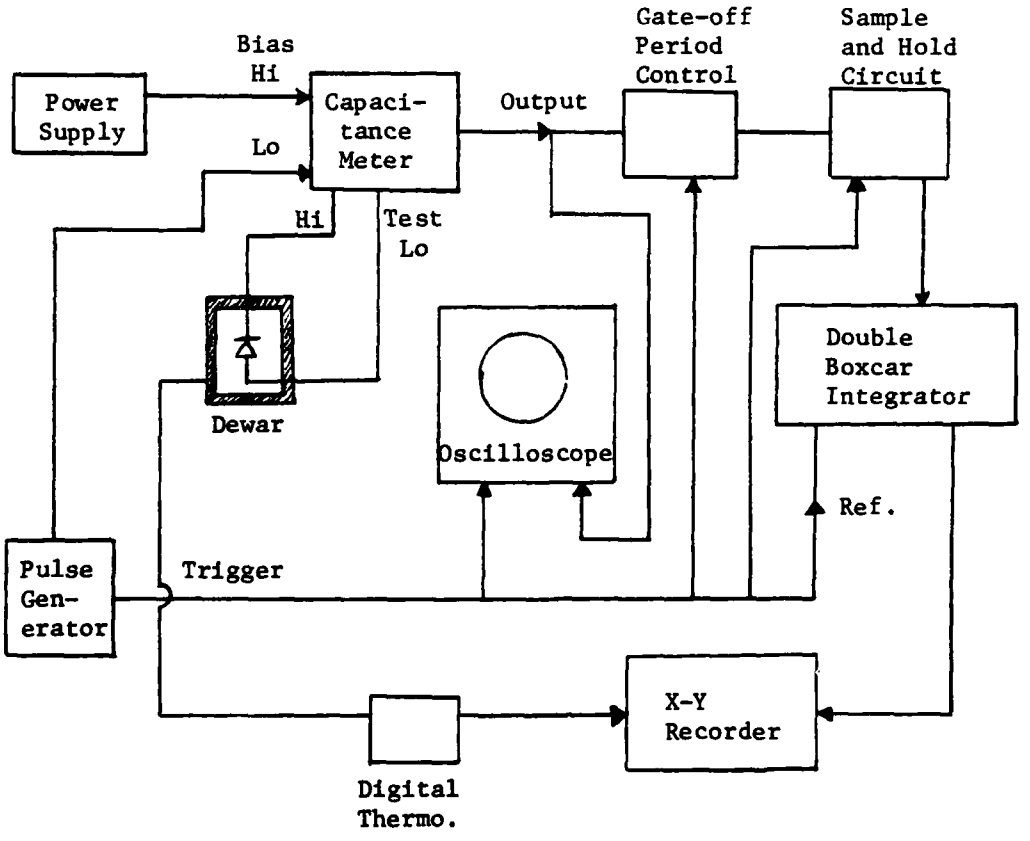


Figure IV-4. Boxcar Integrator DLTS Apparatus

The basic operation of the Boxcar DLTS system is quite complicated but can be simplified to provide a quick understanding of the process. The diode is placed in the dewar with leads connecting it to the Boonton capacitance meter. The power supply provides the reverse bias through the capacitance meter to the sample. The pulse generator provides the majority carrier injection pulse to the diode again through the capacitance meter while triggering the oscilloscope, gate-off period control, sample and hold circuit, and the boxcar integrator. This trigger signal activates the suppression of the capacitance jump that occurs as the depletion region collapses to avoid overloading the Boonton. At this time the boxcar integrator is triggered in order to determine the proper times at which to sample the capacitance transient. The oscilloscope is used to monitor various signal levels important to the proper pulsing of the diode. Important to the analysis of the capacitance transient is the sample and hold circuit which returns the capacitance signal to C_∞ after the boxcar integrator has analyzed it and before the next bias pulse.

The second DLTS setup is located at the U. S. Naval Academy, utilizing a lock-in amplifier for signal analysis. It was built by 2nd Lieutenant Stephen L. Spehn, USMC in 1979-1980 to study DLTS as an experimental technique. A schematic is shown in Figure IV-5. This setup was used to obtain lock-in lineshapes for the initial work in the current study. Specific differences in the signal analysis

of the two systems are given in the sections on signal processing. The basic operation of the system as far as the sequence of events is the same as the boxcar with minor variation.

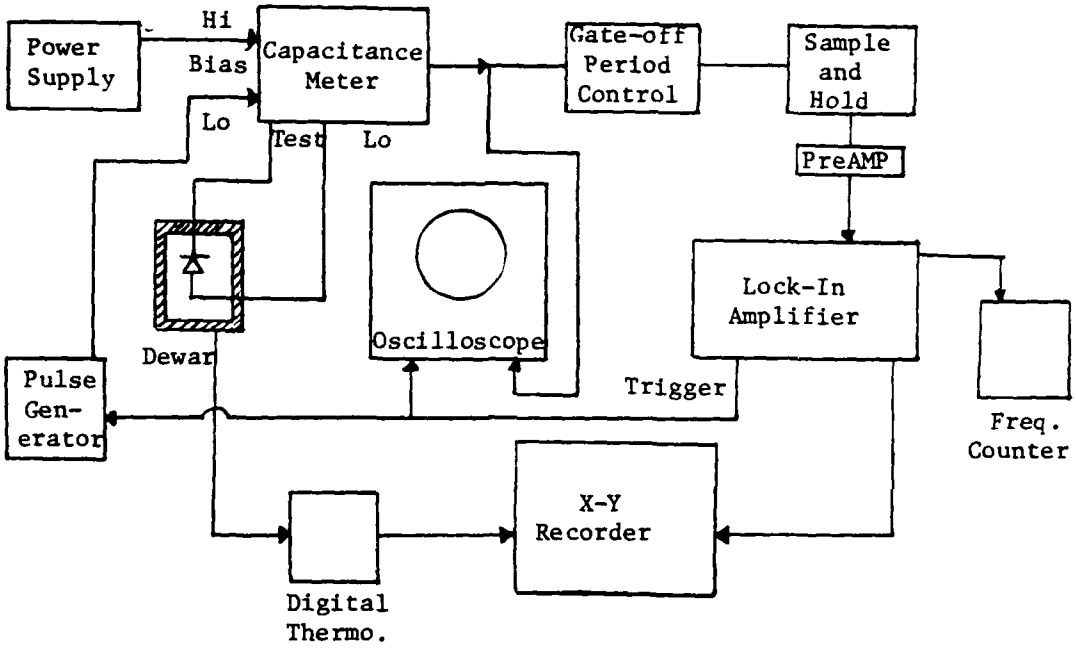


Figure IV-5. Lock-In Amplifier DLTS Apparatus

IV-4. Emission Rate Window

The transient capacitance response of a reverse biased p^+-n diode is the essential physics on which the DLTS technique relies. DLTS is a convenient method by which the important information about trapping states is derived in a short time rather than by tedious examination of capacitance transients at many single temperatures. The device that makes DLTS so powerful is the creation of an

emission rate window. It is within this window that a peak response is achieved by the system to a specific rate of capacitance decay. This peak may be displayed graphically and analyzed for trap parameters by one method common to most literature and another that was extensively used in this study and will be discussed in a later chapter. The emission rate window is currently produced using the two pieces of equipment discussed. The operation of the double boxcar integrator will be discussed first.

IV-5. Boxcar Integrator Signal Analysis

A double boxcar integrator coupled to a fast response capacitance bridge is able to provide averaging to give a good signal-to-noise ratio in order to better detect low concentration traps. A commerical capacitance meter such as the Boonton 72B may be substituted in lieu of a bridge but some response time is sacrificed. Modifications can be made to the Boonton to increase the response time to 100-300 microseconds in comparison to the bridge's response time of 10-30 microseconds. The emission rate window is set by the sampling times at which the boxcar measures the value of the capacitance transient supplied by the capacitance meter. As the temperature is scanned the shape of the transient changes responding to the changing thermal emission rates of the traps. The output of the boxcar is the difference in capacitance of the p^+-n junction at the

different sampling times. It is given by:

$$S(t) = \frac{[C(t_1) - C(t_2)]}{\Delta C(0)} \qquad \text{(IV-5a)}$$

where $\Delta C(0)$ is the change in capacitance caused by the pulse before emission. S(t) is shown in Figure IV-6.

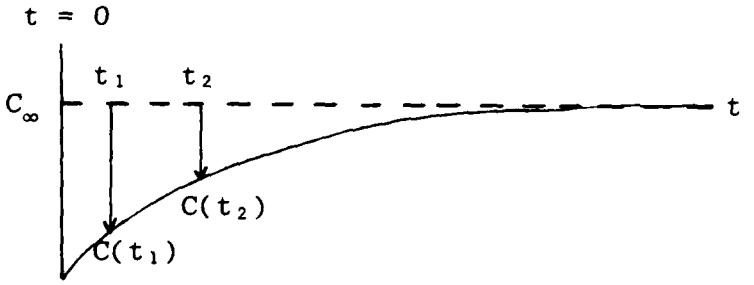


Figure IV-6. Boxcar Sampling Times

The emission rate window may be found by writing the normalized transient as:

$$S(t) = e^{-et_1} - e^{-et_2} \qquad \text{(IV-5b)}$$

where the emission rate is given by Equation IV-1g for a simple single state trap. One may solve for the emission rate at which peak response is obtained (emission rate window) by differentiating Equation IV-5b, setting equal to zero, and solving for e. This gives the emission rate window as a function of the sampling times.

$$e_{max} = \frac{\ell n(\frac{t_1}{t_2})}{t_1 - t_2} \qquad \text{(IV-5c)}$$

By varying the sampling times one may change the emission rate window such that on two thermal scans two different peaks are observed at distinct temperatures. The analysis at a single emission rate is shown in Figure IV-7 as the capacitance transient changes with temperature. The left side shows the transients at different temperature while the right side shows the DLTS peak.[10]

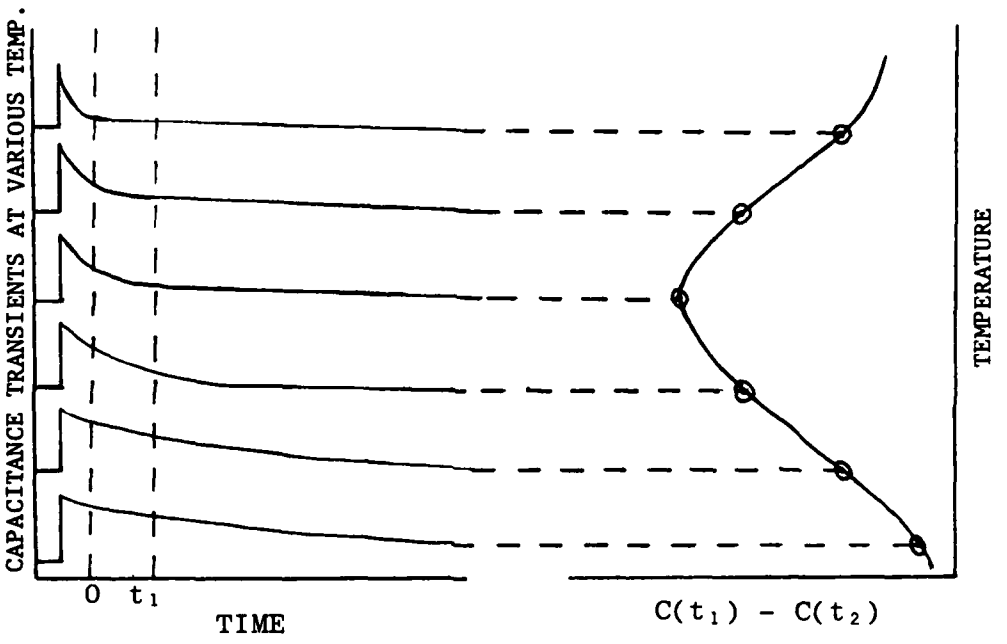


Figure IV-7. Boxcar DLTS Peak Formation

The emission rate window may be changed most successfully by maintaining a constant ratio between t_1 and t_2 while changing both. In this way the shape of the peak is unchanged, only moved over to the new peak response temperature. Less desirable results are obtained when the ratio is not held constant since the peak changes shape and

makes a visual comparison between runs difficult. Changing the emission rate window produces a series of peaks at distinct temperatures for several runs which yields to the classic method of data analysis used by most authors. The emission rate for a simple single state electron trap was derived as Equation IV-1g given by:

$$e = AT^2 e^{-\frac{\Delta E}{KT}} \qquad \text{(IV-1g)}$$

Rearranging and taking the natural logarithm of both sides gives:

$$\ell n\left[\frac{T^2}{e}\right] = \frac{\Delta E}{KT} - \ell n\, A \qquad \text{(IV-5d)}$$

This is an equation of the y = mx + b form. If one plots $\ell n\ \frac{T^2}{e}$ versus 1/T, the slope of the straight line is $\Delta E/K$ from which the trap depth may be found and the intercept is $-\ell n\, A$ which contains among other terms, the capture cross section of the trap. As was mentioned before, doing this type of Arrhenius plot is correct for simple single state traps, but may lead to misleading values of trap parameters for more complicated trapping states. A different method of trap characterization which does not use an Arrenius plot analysis is used in this study. It is theoretically able to determine trap parameters from a single DLTS thermal sweep. This method of fitting the entire DLTS peak by simulating the boxcar output on the computer will be discussed in a later section.

IV-6. Lock-In Amplifier Signal Analysis

The determination of the emission rate window in a DLTS setup using a lock-in amplifier is a rather more strenuous task. The following derivation and analysis is attributed to 2nd Lieutenant Stephen L. Spehn, USMC who developed it as a midshipman.[11] It will be presented here as most of the preliminary data and subsequent synthesis of the DX center ground-excited state model was done using a lock-in system. A representation of the capacitance transient appears as shown below

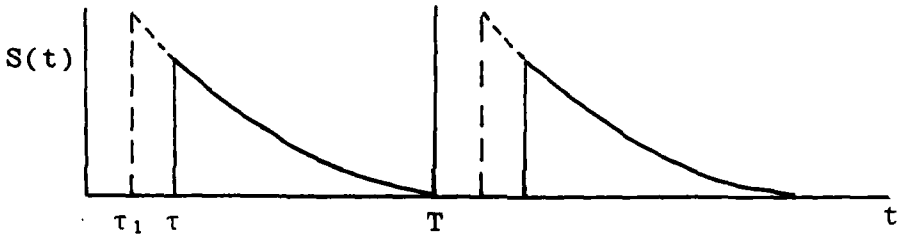


Figure IV-8. Lock-In DLTS Capacitance Transient

where τ_1 is the length of the majority carrier pulse; τ is the length of the system hold time; and T is the system period. The function S(t) is given by:

$$S(t) = \begin{cases} 0 & 0 \le t < \tau \\ e^{e\tau_1} C(0)(e^{-et} - e^{-eT}) & \tau \le t \le T \end{cases} \qquad \text{(IV-6a)}$$

Expanding S(t) into a Fourier Series yields

$$S(t) = \frac{a_0}{2} + \sum_{n=1}^{\infty} [a_n \cos 2\pi n \frac{t}{T} + b_n \sin 2\pi n \frac{t}{T}] \qquad \text{(IV-6b)}$$

where

$$a_0 = \frac{2}{T} \int_0^T S(t)dt$$

$$a_n = \frac{2}{T} \int_0^T S(t)\cos 2\pi n \frac{t}{T} dt$$

$$b_n = \frac{2}{T} \int_0^T S(t)\sin 2\pi n \frac{t}{T} dt$$

The signal is sent through a signal tuned amplifier which for a Fourier Series signal provides a gain which is a function of the order of the harmonic (n). The output is given by:

$$S'(t) = \sum_{n=1}^{\infty} g(n)[a_n \cos 2n\pi \frac{t}{T} + b_n \sin 2n\pi \frac{t}{T}] \qquad \text{(IV-6c)}$$

The output of the signal tuned amplifier is sent through a mixer where it is multiplied by a synchronous square wave given by the Fourier Series:

$$SW(t) = \sum_{n=0}^{\infty} \frac{4}{\pi(2m+1)} \sin[(2m+1)2\pi \frac{t}{T} + \zeta] \qquad \text{(IV-6d)}$$

where ζ is the phase difference between the square wave and the capacitance transient. The output of the mixer is a series of sum and difference components which are sent through a low pass filter with cutoff frequency

$$fc = \frac{1}{8TC} \qquad \text{(IV-6e)}$$

where TC is the time constant set on the front of the lock-in amplifier. The effect of the filter and the highly frequency selective signal tuned amplifier is to screen out all but the fundamental Fourier component of the signal. The lock-in output is then given by:

$$L(T) = \frac{2}{\pi}[a_1 \sin\zeta + b_1 \cos\zeta] \qquad \text{(IV-6f)}$$

Solving for the coefficients and using the definitions

$$\tau = fT \qquad x = eT \qquad \tau_1 = f_1 T$$

the output is given by:

$$L(T) = \frac{2}{\pi} C(0) e^{f_1 x}\left[\left[\frac{2e^{-fx}}{x^2+4\pi^2}(x\cos 2\pi f - 2\pi \sin 2\pi f) - \frac{2x\,e^{-x}}{x^2+4\pi^2} + \frac{e^{-x}}{\pi}\sin 2\pi f\right]\sin\zeta + \left[\frac{2e^{-fx}}{x^2+4\pi^2}(x\sin 2\pi f + 2\pi\cos 2\pi f) - \frac{4\pi e^{-x}}{x^2+4\pi^2} + \frac{e^{-x}}{\pi}(1 - \cos 2\pi f)\right]\cos\zeta\right] \qquad \text{(IV-6g)}$$

The emission rate window is found by taking the derivative of L(T) with respect to x, setting the expression equal to zero, and solving for x. The emission rate window can be selected by referring to the plots of x versus fractional holding time which is the ratio of the gated off signal length to the period of the injection pulse and then setting the corresponding frequency on the front of

the lock-in amplifier. These plots were developed by Spehn and can be found in his report. Perhaps a more practical method is to set the frequency at a convenient value,then determine the emission rate window. The output of the lock-in is a series of peaks which yield to the same Arrhenius plot type of analysis as the boxcar setup with the same misleading results for complex trapping states.

Chapter V

Data Analysis and Modeling of the DX Center

V-1. The Arrhenius Plot

In the initial phases of the research a lock-in amplifier DLTS system built by Spehn was used. The data obtained was of excellent quality and yielded well to the Arrenius plot discussed previously. It was possible to obtain the value of the trap depth and prefactor from many samples with ease. Some problems occurred in determining the actual phase shift of the lock-in signal but these were solved and the correct procedure for setting zero phase shift in the lock-in is available in the Appendix. A problem was encountered though that has led to a different model of the DX center in GaAℓAs.

An Arrhenius plot of $\ell n\ T^2/e$ versus $1/T$ uses only the position of the peak in its analysis. It was noticed that examining the entire lineshape did not yield results consistent with the known output of a DLTS run on a simple single state electron trap. Comparing the full widths at half maximum showed that all of the experimental data curves were much broader than theoretical curves created by computer simulation of lock-in or boxcar output. The broader data curves could not be created by the action of simple single state traps exponentially emitting electrons to the conduction band. A simple single state is shown below.

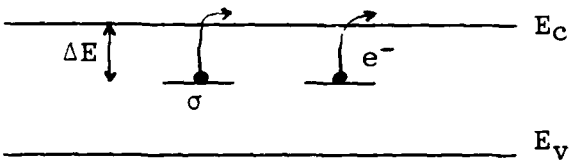


Figure V-1. Simple Single State Electron Trap

The emission rate of the trap is given by the relationship previously derived from the Law of Detailed Balance. No combination of prefactor A or trap energy, especially those calculated from an Arrhenius plot, could generate the wide peaks that were observed. Arrhenius plots yielded the following values for trap parameters taken from the data runs on the GaAℓAs samples discussed in Chapter III.

Semiconductor	Energy Depth (eV)	Prefactor
S-214-BA1	.271	1.74×10^7
S-214-BB1	.284	3.34×10^7
L-107-C1A,1	.288	3.25×10^7

Table V-1. Arrhenius Analysis of DX Center

A DLTS peak obtained from a known simple state in silicon was easily fit using Arrhenius plot values for prefactor and energy showing that this type of analysis yields accurate values for these states. The broad peaks of the DX center lead one to believe that the peaks may be more

accurately characterized by fitting the entire curve with an appropriate model reflecting the complex nature of the trap.

V-2. The Ground-Excited State Model

A model of deep electron traps proposed by G. J. Rees and H. G. Grimmeiss consists of a communicating ground plus excited state.[12] In this model, carrier capture via an excited state into the ground state and their subsequent re-emission is offered as an explanation for increased capture cross section with temperature. No mention is made though in the article that this capture and emission mechanism produces DLTS peaks characteristically wider than simple traps. A schematic of this model is shown below with the relevant electron emission rates indicated.

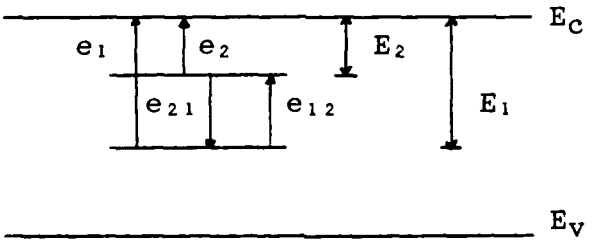


Figure V-2. Ground-Excited State Electron Trap

The direct filling of the ground state from the conduction band is neglected since the large capture cross section of the excited state effectively eliminates this process.

The proper analysis of this model includes solving the coupled rate equations between the communicating states and the conduction band. Through detailed balance arguments one gets the thermal emission rates of each process shown in Figure V-2.

$$e_1 = A_1 T^2 e^{-E_1/KT} \qquad \text{(V-2a)}$$

$$e_2 = A_2 T^2 e^{-E_2/KT} \qquad \text{(V-2b)}$$

$$e_{12} = A_3 e^{-(E_1-E_2)/KT} \qquad \text{(V-2c)}$$

$$e_{21} = A_3 \qquad \text{(V-2d)}$$

The transient electron occupation probabilities of the traps are proportional to the thermal emission rates and the probability that a trap is occupied. These transient occupation probabilities can be expressed as below,

$$\frac{df_1}{dt} = a_{11} f_1 + a_{12} f_2 \qquad \text{(V-2e)}$$

$$\frac{df_2}{dt} = a_{21} f_1 + a_{22} f_2 \qquad \text{(V-2f)}$$

where f_1 and f_2 are the occupation probabilities of the ground and excited states, respectively. The coefficients are functions of the individual thermal emission rates given in Equation (V-2a-d). Solving these two equations

simultaneously yields occupation probabilities as a function of time given by:

$$f_1 = A_{11}e^{w_1 t} + A_{12}e^{w_2 t} \qquad \text{(V-2g)}$$

$$f_2 = A_{21}e^{w_1 t} + A_{22}e^{w_2 t} \qquad \text{(V-2h)}$$

where w_1 and w_2 are complicated functions of the thermal emission rates. The coefficients are again functions of the thermal emission rates plus terms reflecting the initial filling ratio of the ground and excited states. A complete treatment of this derivation with all constants defined is given in the Appendix.

DLTS essentially measures the charge state of the trap and is unable to distinguish between an electron in the ground or excited state. Stated in another way, DLTS measures whether a trap is occupied or empty. This shows that the interesting quantities are the occupation probabilities given in Equations V-2g,h. During a majority carrier injection pulse in which the depletion region is collapsed, electrons are captured into the excited state and if the pulse width is large enough as it was in all data runs, it will fill the ground and excited states in accordance with the thermodynamic equilibrium ratio.

$$\frac{f_1}{f_2} = \frac{1}{1 + e^{(E_1 - E_2)/KT}} \qquad \text{(V-2i)}$$

At all temperatures and pulse widths used, conditions were met such that most electrons had dropped to the ground state before the trap was allowed to emit. At t = 0, the end of the injection pulse, the coefficients in Equations V-2g,h reflect this equilibrium ratio. The transient capacitance of the trap is then given by some combination of the exponentials in the occupation probabilities and thus the signal output of a boxcar DLTS system is given by:

$$S(t) = [f_1(t_1) + f_2(t_1)] - [f_1(t_2) + f_2(t_2)] \quad (V\text{-}2j)$$

where the charge states of the traps are directly proportional to the junction capacitance of the diode. Hence, the signal out is the change in occupation of the trap with time which results in the change in the capacitance of the diode as shown in Chapter IV. By sweeping temperature a different change in capacitance is found between the two sampling times t_1 and t_2 for different temperatures. When the combination of exponential emission rates matches the emission window a peak results. This is a crucial point in that any type of trap with an exponential emission rate within the emission window and by consequence, the right trap parameters, will produce a peak at the same temperature no matter what the structure of the trap is. This is where the Arrhenius plot breaks down. In order to gain tangible evidence that the DX center in GaAlAs has a complex ground-excited state structure one has to fit the entire data peak to include the details of inter-communication and emission rates.

V-3. Computer Simulation and Trend Studies

Computer programs were written simulating the output of both types of DLTS setups. The important variable trap parameters in these simulations were the energies and prefactors in the emission rate equations V-2a-d. For typical values of prefactors and trap energy levels, broader peak widths than could be expected from simple single states were generated. Several trend studies were done to determine the effect on the shape (primarily width) and the position of the peak when the prefactors and energies were changed independently. The results of these studies will now be presented graphically with comments.

The effect on the shape and position of the DLTS peak due to the manipulation of trap parameters is important in that this knowledge may be useful when shaping theoretical parameters to experimental data. Several definite trends were observed when the energies of the two trap levels were changed. Increasing the energy gap between the ground and excited states with the ground state fixed, shifts the peak to slightly higher temperature and also narrows the FWHM against the tendency to be broader at higher temperature. This case is analogous to placing the excited state closer to the conduction band and is shown in Figure V-3. The second trend study on energy levels is the case in which the energy gap is widened by holding the excited state fixed and moving the ground state deeper into the band gap.

An increased ΔE by this method again moves the peak to higher temperature, but with more noticeable effect as seen in Figure V-4. The characteristic broadening of the peak is observed here with higher temperature. The third manipulation of the energy is the moving of the entire state deeper into the band gap with energy level separation held constant. This has similar effects as the last case with the peak moving to higher temperature with the characteristic broadening (see Figure V-5).

Trend studies on prefactors and consequently, the values of a trap capture cross section, were also performed to become familiar with the effects of these parameters. Decreasing the capture cross section of the ground state as seen in Figure V-6 has the effect of shifting the peak to higher temperature combined with the lifting of the leading (low temperature) edge of the peak resulting in a broader than expected asymmetric peak. Note the loss of symmetry in the extremes of Figure V-6. Interestingly, increasing the capture cross section of the excited state in Figure V-7 does not shift the peak, but only lifts the leading edge contributing to the width and asymmetry of the peak. Note that decreasing the ground state's capture cross section had the same effect plus a shift. The last case of a single parameter contributing to a trend is when the prefactor on the communication rate between the states is changed. Looking at Figure V-8 one sees that this single parameter has the most profound effects. The most important

aspect of the trends going on is that the communication prefactor must be somewhere in between 1×10^4 and 1×10^6 to produce a broad peak. The other effect clearly evident is the change in shape of the leading and trailing edges with increasing communication prefactor.

The mechanism by which changes in energy or capture cross section manifest themselves as changes in peaks may be comprehended by understanding that an electron in a trap has several competing paths of emission back to the conduction band. By increasing or decreasing some parameter in the emission relationships one is favoring one path over another. A particular emission path determines the time constant of the capacitive transient and therefore determines the shape of the DLTS peak. This property makes the trend study a valuable tool in the process of fitting a peak and characterizing a trap's parameters.

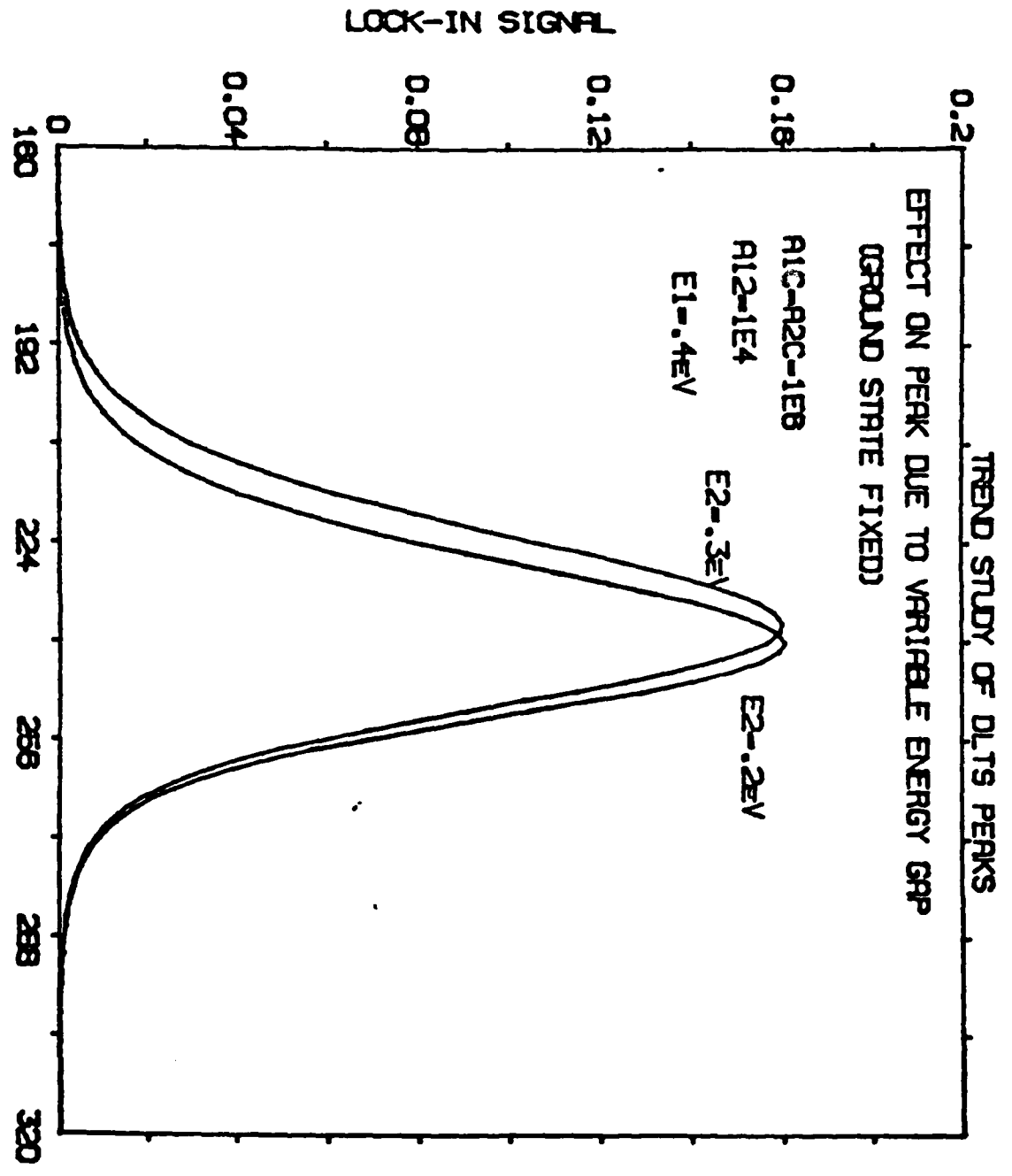

TREND STUDY OF DLTS PEAKS
EFFECT ON PEAK DUE TO VARIABLE ENERGY GAP
(GROUND STATE FIXED)
A1C-A2C-1E8
A12=1E4
E1=.4eV
E2=.3eV
E2=.2eV
LOCK-IN SIGNAL
0
0.04
0.08
0.12
0.16
0.2
180
192
224
256
288
320
TEMP (K)

Figure V-3

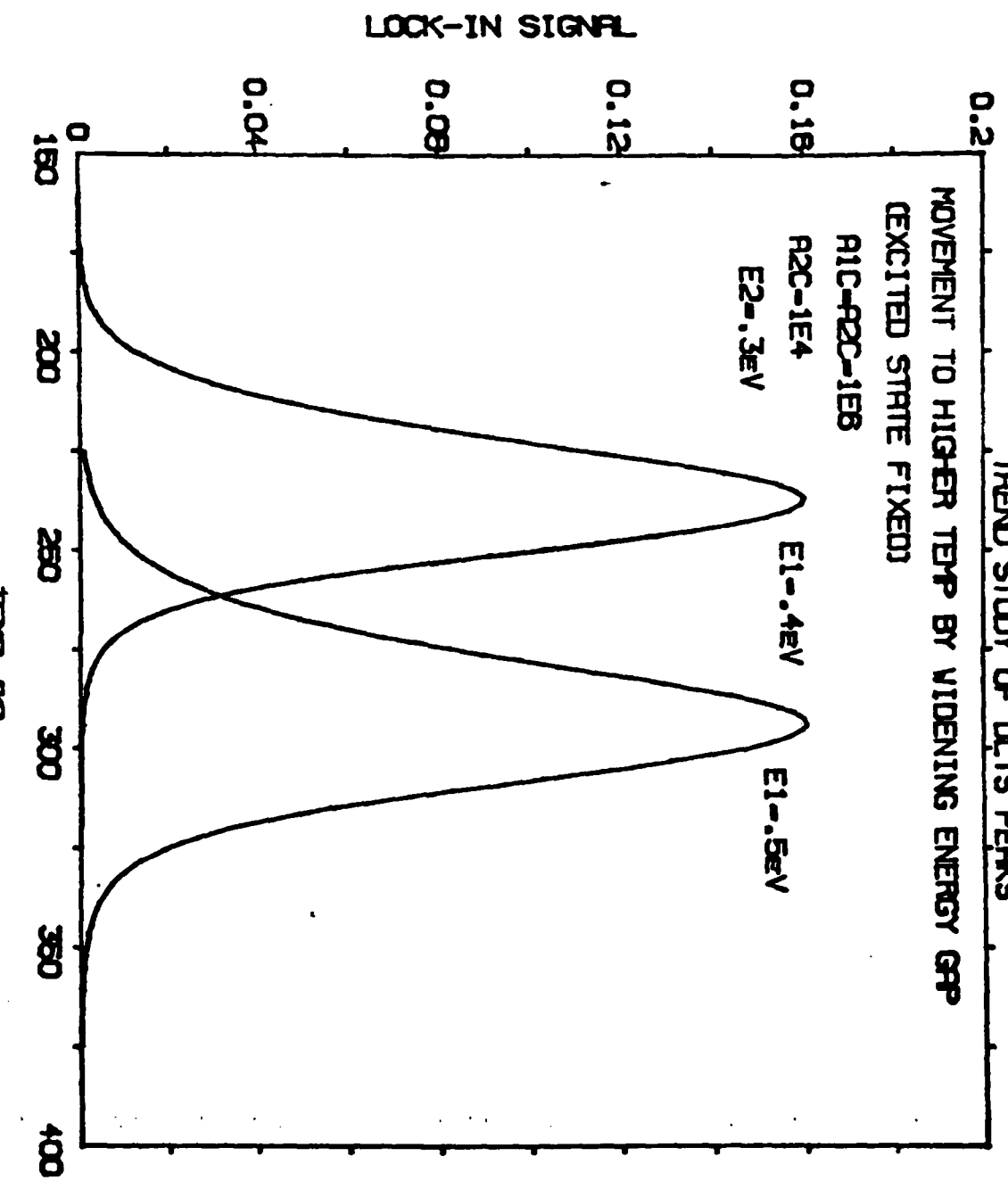

TREND STUDY OF DLTS PEAKS
MOVEMENT TO HIGHER TEMP BY WIDENING ENERGY GAP
(EXCITED STATE FIXED)
A1C-A2C=1E8
A2C=1E4
E2=.3eV
E1=.4eV
E1=.5eV
LOCK-IN SIGNAL
0.2
0.16
0.12
0.08
0.04
0
150
200
250
300
350
400
TEMP (K)

Figure V-4

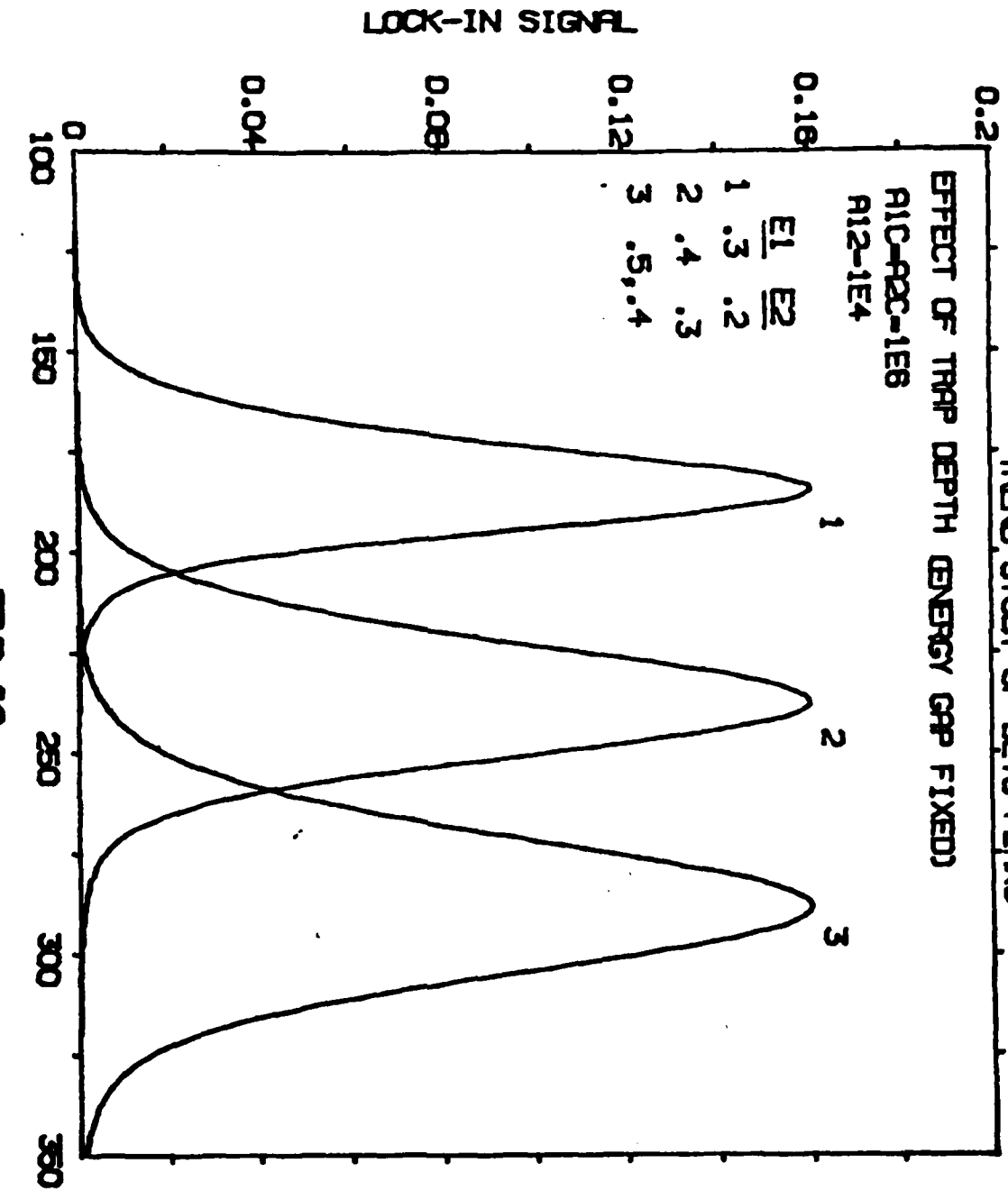

TREND STUDY OF DLTS PEAKS
EFFECT OF TRAP DEPTH (ENERGY GAP FIXED)
A1C-A2C=1E6
A12=1E4
E1 E2
1 .3 .2
2 .4 .3
3 .5,.4
LOCK-IN SIGNAL
0.2
0.16
0.12
0.08
0.04
0
100
150
200
250
300
350
TEMP °K
1
2
3

Figure V-5

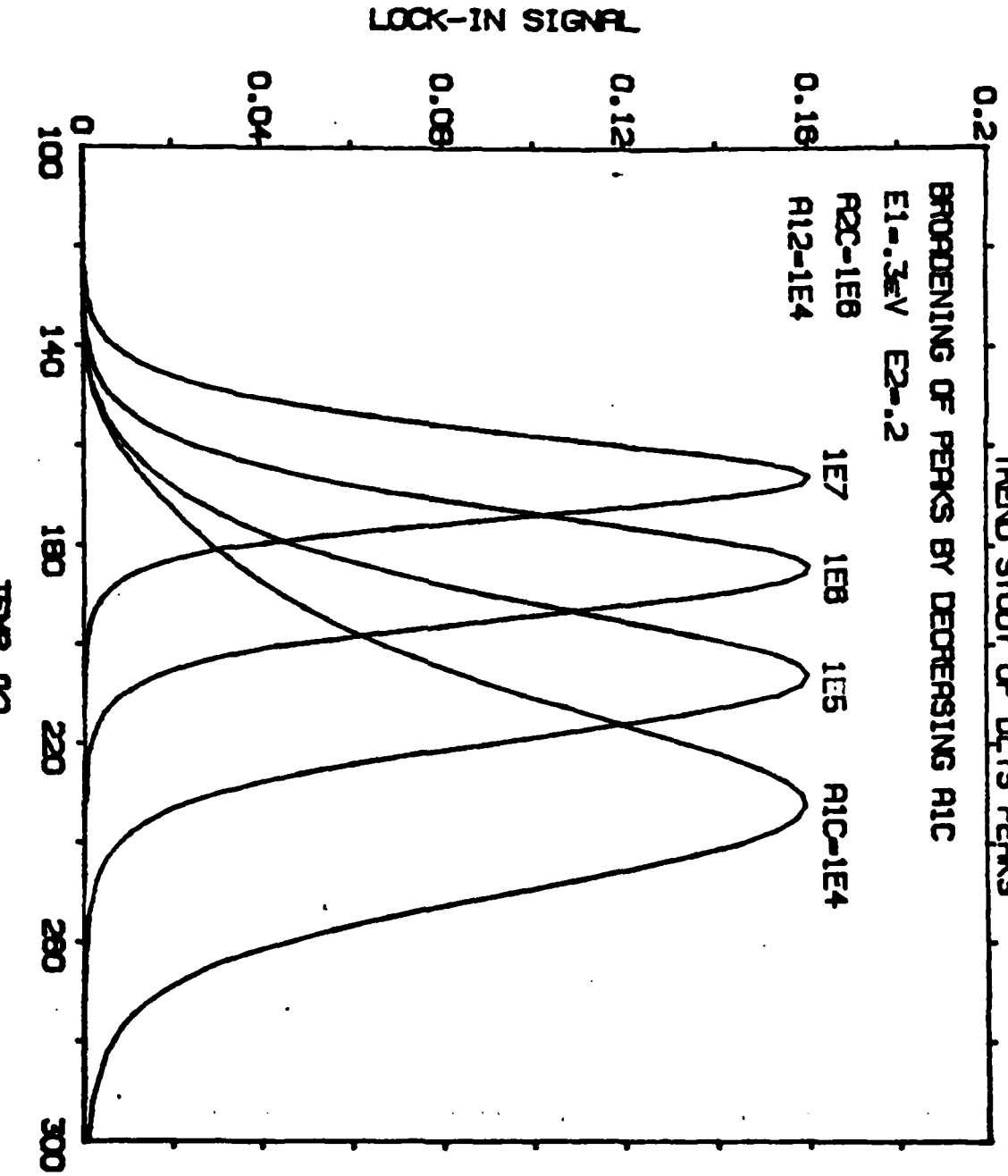

TREND STUDY OF DLTS PEAKS
BROADENING OF PEAKS BY DECREASING A1C
E1=.3eV E2=.2
A2C=1E8
A12=1E4
1E7
1E8
1E5
A1C=1E4
LOCK-IN SIGNAL
0
0.04
0.08
0.12
0.16
0.2
100
140
180
220
260
300
TEMP OK

Figure V-6

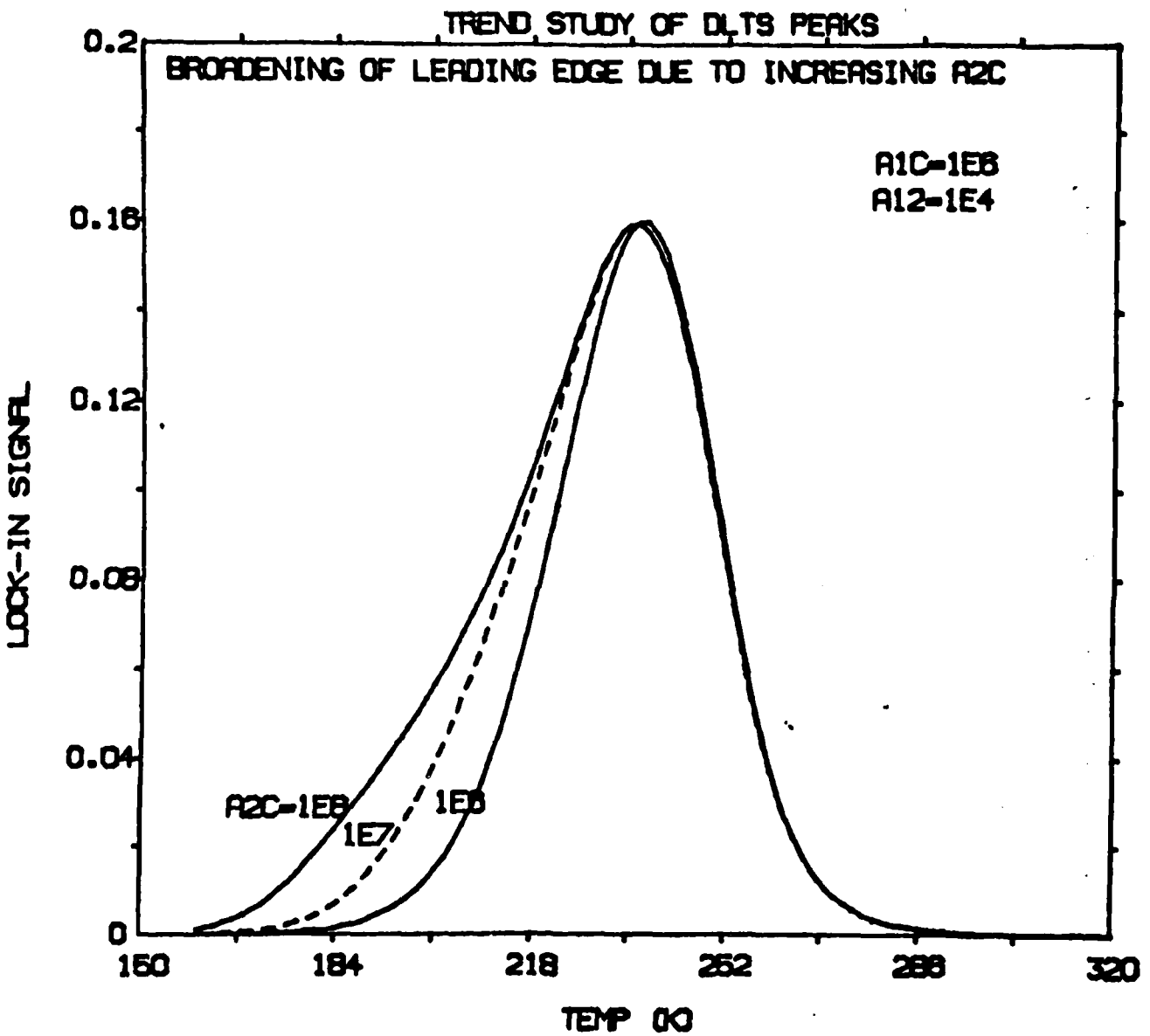

TREND STUDY OF DLTS PEAKS
BROADENING OF LEADING EDGE DUE TO INCREASING A2C
A1C=1E8
A12=1E4
LOCK-IN SIGNAL
0.2
0.16
0.12
0.08
0.04
0
A2C=1E8
1E7
1E6
150
184
218
252
286
320
TEMP OK

Figure V-7

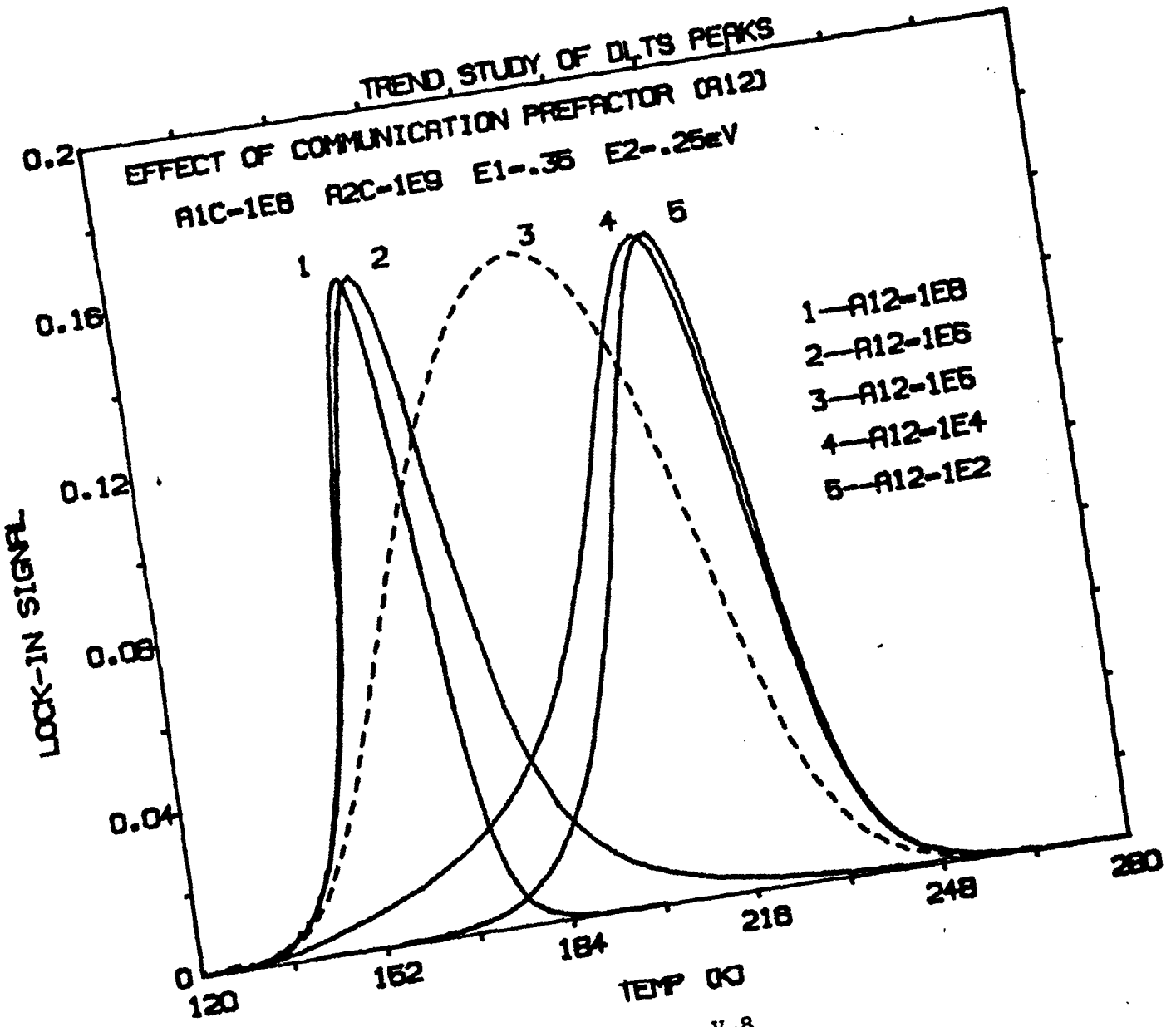

TREND STUDY OF DLTS PEAKS
EFFECT OF COMMUNICATION PREFACTOR (A12)
A1C-1E8 A2C-1E9 E1-.35 E2-.25eV
1
2
3
4
5
1—A12-1E8
2—A12-1E6
3—A12-1E5
4—A12-1E4
5—A12-1E2
LOCK-IN SIGNAL
0.2
0.16
0.12
0.08
0.04
0
120
152
184
216
248
280
TEMP OK

Figure V-8

V-4. Curve Fitting and Trap Parameters

After performing the trend studies on a DLTS signal from a lock-in amplifier, data for a GaAℓAs sample was obtained from Richard Magno at NRL using a double boxcar integrator. The system at NRL has much better noise filtering capability than the lock-in setup and the data obtained was of unusually excellent quality. Specifics of the samples were discussed in Chapter III. The data was digitized using a Tektronix 4051 terminal mated to a Tektronix 4956 digitizing tablet. The actual data fitting was done by inserting the function written in APL describing the output of a boxcar integrator as it analyzes the transient capacitance signal of the DX center into a program written by Major R. J. Kimble, USMC. This program, modified by Professor C. W. Rector, will fit a set of points to any function specified with limitations on the number of parameters used solely depending on the run time available. The program is listed in the USNA computer library under "APLLIB***: FITFN." The program is easily run with instructions provided as needed.

To validate the fitting procedure, data files of theoretical peaks were created from computer simulations of various types of trap models. This data was fitted using the known parameters and received "best fit" parameter values within a very close range of what were expected. Another purpose of this exercise was to visually see using the

graphics display what a good fit could be expected to look like. The fits for a computer simulated simple single state and a ground-excited state trap are contained in the Appendix.

The ground-excited state model plots showed all the characteristics of the shape of the data curves, most importantly, the correct FWHM. Six parameter fits were done on three sets of data runs of three different GaAℓAs samples. The parameters were the energies of the ground and excited states, the prefactors containing capture cross section information of the two levels, the communicating prefactor, and a normalizing term to adjust the magnitude of the fit to the data. A sample fit on the DX center in GaAℓAs is shown in Figure V-9. Each curve was fit resulting in the parameter values shown in Table 1. The values are fairly close when comparing them in pairs realizing that each peak is at a different temperature due to the changed emission rate window. Representative samples of fitted curves are included in the Appendix.

An Arrhenius plot of the DX center data gives a value for a single prefactor and energy different from any type of average values calculated from the curve fitting technique. Presented in Table 2 are the Arrhenius plot values and the logarithmic averages of the prefactors determined by curve fitting.

```
F5 =    12036600.
F6 = 219779000.
F7 =      200386.
E1 =     0.297107
E2 =     0.209493
A5 =      4.08412
RMS ERROR:
   0.0375792

BOX2G .005  .01
```

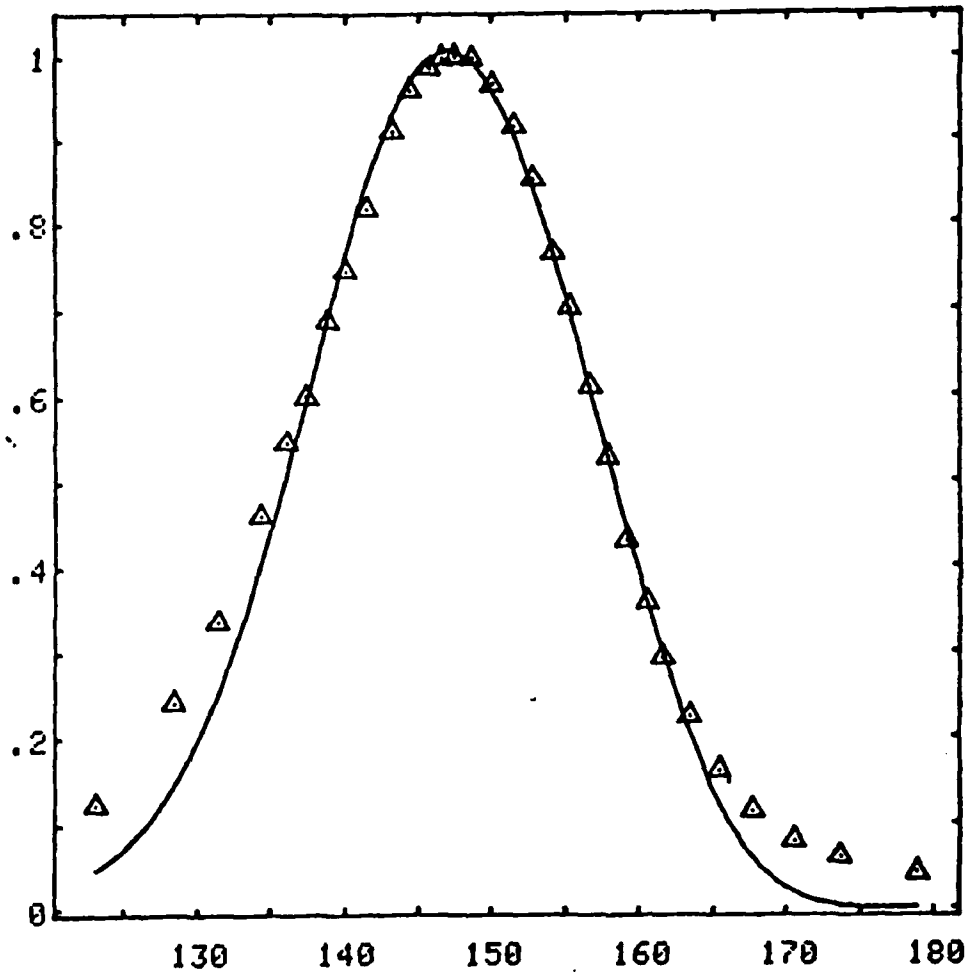


Figure 9. DX Center Fitted to Ground-Excited State Model

SAMPLE	RUN	A1Cx10^6	A2Cx10^8	A12x10^5	E1(eV)	E2(eV)
S-214-BA1	A	7.657	1.236	7.537	.282	.221
	B	8.160	2.106	9.237	.283	.209
	C	8.053	2.117	9.213	.289	.211
	D	7.015	2.183	8.641	.291	.207
	E	7.006	2.230	9.304	.292	.200
	F	6.993	2.216	9.580	.291	.193
	G	7.098	2.229	9.538	.293	.189
S-214-BB1	A	13.00	1.660	5.720	.299	.240
	B	14.37	2.520	4.532	.299	.239
	C	9.692	1.948	3.627	.298	.237
	D	10.47	1.948	3.522	.299	.229
	E	9.379	4.383	3.344	.309	.235
	F	10.60	2.194	2.300	.298	.218
	G	12.04	2.198	2.004	.297	.209
L-107-C1A,1	A	10.33	1.293	6.666	.296	.232
	B	11.42	1.328	3.605	.290	.214
	C	11.18	2.557	3.668	.303	.234
	D	12.93	2.374	3.790	.305	.225
	E	13.01	2.398	3.064	.301	.213
	F	13.81	3.349	2.065	.308	.225
AVERAGE:		10.21x10^6	2.223x10^8	5.578x10^5	.295	.219

A1C - Ground State Prefactor
A2C - Excited State Prefactor
A12 - Communication Prefactor
E1 and E2 - Ground and Excited State Energy

Table 1 - Best Fit Trap Parameter Values

	ARRENIUS VALUES		CURVE FIT VALUES	
SAMPLE	E(eV)	PREFACTOR	E(eV)	PREFACTOR
L-107-C1A,1	.288	3.245×10^7	.262	1.862×10^7
S-214-BB1	.279	2.460×10^7	.265	1.100×10^7
S-214-BA1	.268	1.350×10^7	.247	1.110×10^7

Table 2 - Comparison of Analyses

On first comparison of the values, they do not look that much different. However, one has to be very careful since the width and position of a peak is extremely sensitive to the parameters. The best way to see this is to plot a simulated single state peak using the Arrhenius values and compare it to one of the DX center data peaks. This is done in Figure V-10. Trying to fit the DX center data with a simple single state emission function is also not possible no matter what values one uses for prefactor and energy. The broadened peak is not a characteristic of a single state trap. Conversely, data from a known single state may be fitted by a ground-excited state trap function by making the capture cross section of the ground state large compared to the excited state, or vice versa and eliminating the communication between the two states. These steps allow the complicated trap to simulate a simple one. However, the values of the parameter do not make sense when one considers the actual physical situation.

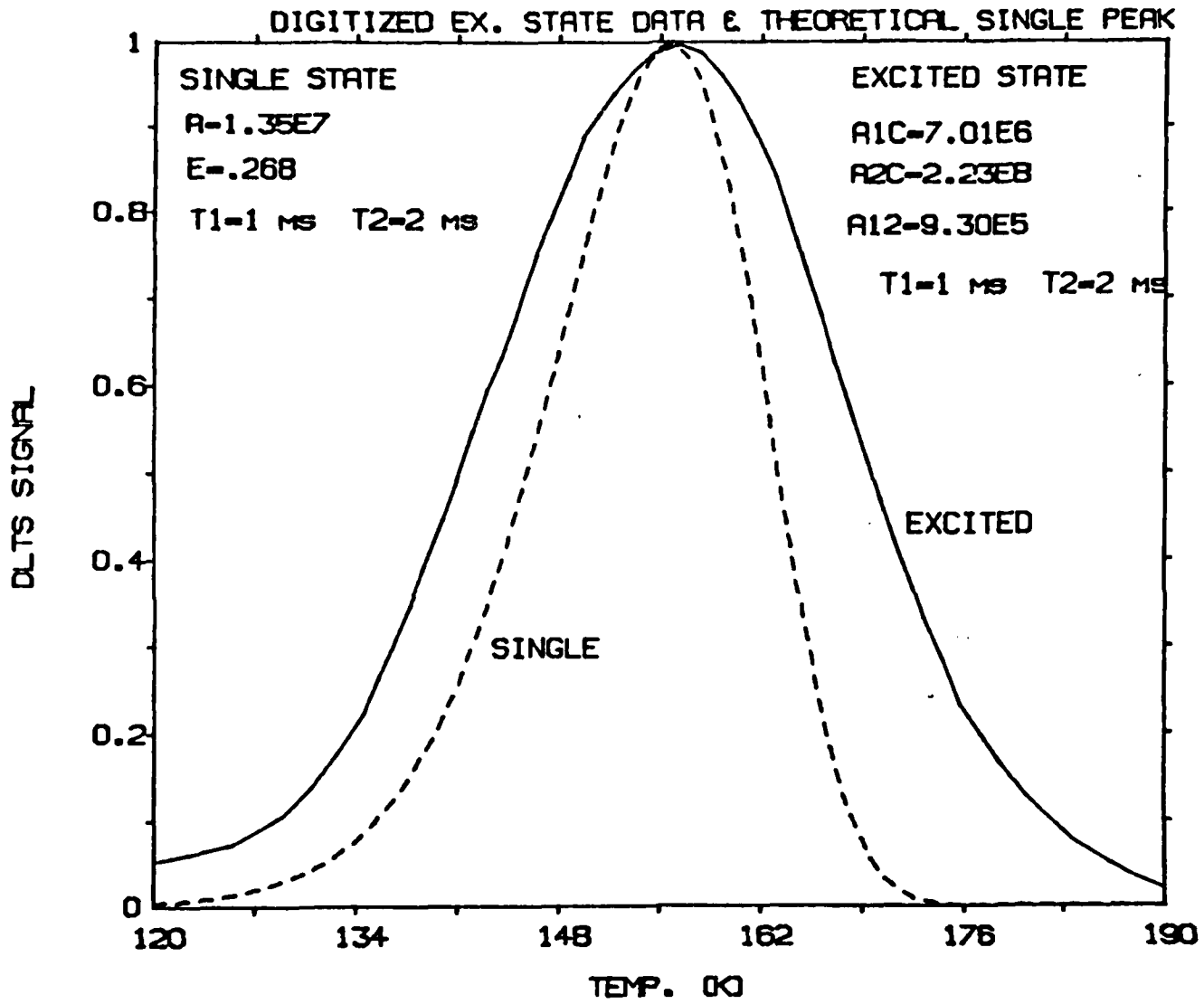


Figure 10. Comparison Between DX Center Data and Simulated Single State

Based on this curve fitting technique, the ground-excited state model of the DX center explains many features of the DLTS peaks obtained. All of the fits have their peaks corresponding to the peak of data. The width of the fit is correct and as can be seen by examining the plots, all the data points fall very close to the generated curve. Minor deviations from the fit on the wings of the peak could be caused by uncertainty in placing the baseline on the actual data when digitizing the peaks. Noise and differences in the observed baseline from the low to high temperature sides are the source of this uncertainty. How accurately the thermocouple can follow a temperature sweep may shift the curve to some degree. The magnitude of this shift is known to be about 2K for the data used here. This lag is small enough to be within error limits for the curve fitting analysis. Another feature of the data shown by the complex model is that the inflection points on the sides of the peaks are accurately reflected in the fits. The evidence examined so far has pointed to the fact that the DX center in GaAℓAs could be a complex ground-excited state trap.

V-5. Modeling Problems

Although the DX center data is fit well by the ground-excited state model on a peak-to-peak basis, there are some features that the model cannot explain at the

time of this writing. Theoretically one should be able to take a unique value for each parameter and fit each curve reasonably well, independent of the emission rate window that has been set. This has not been the case with the data presented. When a "best fit" is obtained using the fitting program there may not be a unique local minimum. The program computes many fits by varying each of the six variable parameters then selects the one with the least difference from the data points. The computer searches over this six-dimensional landscape for an absolute minimum but can get stuck in a local minimum giving the resulting parameters for "best fit" values. It was found that this is in part true since the resulting values depended somewhat on the starting parameter values and sensitivity of the search. A combination of initial parameters and sensitivity vectors may result in erroneous "best fit" values. This software contribution to unexplained problems is a possibility although it is not likely in this data, as much care was taken in the selection of initial parameter values, the sensitivity vectors were kept constant, and visual checks were made on the graphic display of the fit.

By careful examination of the parameters in Table 1, one sees a trend in the energy of the excited state on the two samples with a sampling ratio of 2. With decreasing temperature the excited state rises toward the conduction band with surprising regularity. Other not quite as

pronounced trends occur with the prefactor values. The only thing that changed while fitting the peaks was the temperature at which the peak occurred. The model presented here presumes that the prefactors of the emission rates and the energies of the trap levels are independent of temperature. Modifications were made to the fitting function to reflect a first order approximation that the parameters were linear functions of temperature. The results of this were unsatisfactory as the trailing edges of peaks were chopped off. A modification as to what kind of temperature dependence the fitting parameters may have might solve the discrepancy in fitting all of the DLTS peaks at once, but as of this time the dependence has not been found.

A second feature of the data not explained by the original ground-excited state model is the shape of the transient capacitance decay curves. According to this model as presented in Section V-2 the capacitance of the p^+-n junction is proportional to the occupations of the ground and excited states given by:

$$f_1 = A_{11}e^{w_1 t} + A_{12}e^{w_2 t} \qquad \text{(V-2g)}$$

$$f_2 = A_{21}e^{w_1 t} + A_{22}e^{w_2 t} \qquad \text{(V-2h)}$$

The transient capacitance is then given by:

$$C(t) \alpha (A_{11} + A_{21})e^{w_1 t} + (A_{21} + A_{22})e^{w_2 t} \qquad \text{(V-5a)}$$

From the definition of w_1 and w_2 in the Appendix, it is seen that $e^{w_1 t}$ is a slow decay while $e^{w_2 t}$ is a rapid decay. Table 3 is a list of w_1 and w_2 at various temperatures for typical energy and prefactor values.

TEMP. (K)	w_1 (s^{-1})	w_2 (s^{-1})
200	-40.5	-1.00×10^6
210	-134.0	-1.02×10^6
220	-396.8	-1.04×10^6
230	-1061.0	-1.09×10^6
240	-2577.7	-1.18×10^6

Table 3 - Inverse Time Constants
For Bi-Exponential Decay

For the transient capacitance at 220 K the time constant for w_1 and w_2 are 2.52 milliseconds and .000096 milliseconds. From this one can see that the second exponential contributes to the decay transient for only a very brief time. This is true when the coefficient of the fast exponential is not large compared to the coefficient of the slow exponential, which is known to be the case with the data obtained. Graphically this means that the capacitive transient should be displayed by a single exponential. Actual data curves do not display this single exponential feature, but show a combination of two exponentials. The faster of the two is definitely not the fast transient discussed above since its time constant is

far too large. This bi-exponential decay is not a consequence of the possible temperature dependence of the trap parameters because the decay takes place at a single temperature whereas the DLTS peak height is a function of temperature. As of this writing the model proposed for the DX center in GaAℓAs cannot explain this bi-exponential capacitance transient.

Chapter VI

Summary

The DX center in GaAℓAs is best represented at this time by a complex trap structure consisting of a ground and a single excited state. One may be easily misled by the ease with which the simple single state theory, Arrhenius plot analysis can be applied to the DX center with apparently excellent results. However, any kind of DLTS peak created by a single state trap is far too narrow to fit the DX center data although their maximum values may coincide. Modifications to the single state trap theory were made with no success. In a first approximation, making the trap parameters linear functions of temperature could not produce the characteristically broader peaks of the DX center. Phonon broadening of the single state into a Gaussian distribution of states about the original level also could not produce satisfactory lineshapes. The ground-excited state trap model was the only model to produce the broad data peaks of the DX center.

Another important result of this study is the fact that a DLTS lineshape is extremely sensitive to the values of the energy and capture cross sections used in the ground-excited state trap model. A sensitive balance exists between competing paths an electron may take to the conduction band in a complex trap structure. Changing one parameter can radically change the most favored emission path and

therefore the response of the diode to an input signal.

In summary, the analysis of DLTS signals must be a careful process in which the entire lineshape must be fit within reasonable limits. Short-cut techniques such as the Arrhenius plot are extremely useful when applied to simple single state electron traps. Otherwise, the Arrhenius plot is useless in the proper characterization of complex trapping states and can be very misleading. A model of the trap must be proposed and examined to determine whether it can produce DLTS peaks with the major features of the data. This was the technique used to characterize the DX center in GaAlAs.

References

[1]D. V. Lang, "DLTS: A New Method to Characterize Traps in Semiconductors," J. App. Phys., 45 (1974), 3023.

[2]G. L. Miller, D. V. Lang, and L. C. Kimerling, "Capacitance Transient Spectroscopy," Ann. Rev. Mat. Sci., (1977), 391.

[3]D. V. Lang, J. App. Phys., 45 (1974), 3023.

[4]Ibid.

[5]D. V. Lang, Inst. Phy. Conf. Ser. No. 31, (1977), 70.

[6]Ibid., 71.

[7]Ibid., 72.

[8]Ibid.

[9]Jacques E. Ludman and Welville B. Nowak, "Traps in Fast-Neutron Irradiated GaAs Schottky Diodes," Solid State Electronics, 19 (1976), 759.

[10]D. V. Lang, J. App. Phys., 45 (1974), 3026.

[11]Stephen L. Spehn, "Deep Level Transient Spectroscopy As An Experimental Technique," Diss. U. S. Naval Academy 1980, pp. 24-7.

[12]G. J. Rees and H. G. Grimmeiss, "Capture, Emission and Recombination At A Deep Level Via An Excited State," J. Phys. C: Solid State Physics, 13 (1980), 6157.

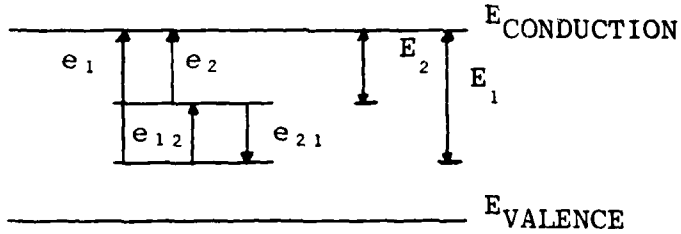
APPENDIX

Procedure for Setting Zero Phase Shift for the Lock-In Amplifier

The following procedure is applicable to the Princeton Applied Research Type A Lock-In Amplifier.

1. Connect CALIBRATE OUT to INPUT A.
2. Set Lock-in frequency to desired value.
3. Turn meter selector switch to MONITOR OUT.
4. Set phase dial to zero.
5. Adjust FREQ. TRIM to obtain a meter maximum.
6. Set outer phase dial to 90°.
7. Adjust phase dial to obtain a meter minimum.
8. Reset outer phase dial to 0°.
9. Reconnect original lines.

Solution of Ground-Excited State Coupled Rate Equation



The emission rates are given by:

$$e_1 = F_5 T^2 e^{-E_1/KT} \qquad e_2 = F_6 7^2 e^{-E_2/KT}$$

$$e_{12} = F_7 e^{-(E_1-E_2)/KT} \qquad e_{21} = F_7$$

The transient occupation probabilities are given by the differential equation

$$\frac{df_1}{dt} = a_{11} f_1 + a_{12} f_2 \qquad \text{(A-1)}$$

$$\frac{df_2}{dt} = a_{21} f_1 + a_{22} f_2 \qquad \text{(A-2)}$$

where

$$a_{11} = -(e_1 + e_{12}) \qquad a_{12} = e_{21}$$

$$a_{21} = e_{12} \qquad a_{22} = -(e_2 + e_{21})$$

To get an expression for the output of a double boxcar integrator for this trap one must solve for f_1 and f_2 which added together is the charge state of the trap.

The solution for f is of the form

$$f_i = A_{i1}e^{w_1 t} + A_{i2}e^{w_2 t} \qquad \text{(A-3)}$$

plugging in this expression for f_1 and f_2 and solving the simultaneous equation in terms of a_{11}, a_{12}, a_{21}, and a_{22} one obtains

$$w_1 = w_2 = N \pm \sqrt{N^2 - \beta}$$

where $N = \frac{1}{2}(a_{11} + a_{22})$

and

$$\beta = a_{11}a_{22} - a_{12}a_{21}$$

let $w_1 = w_+$ and $w_2 = w_-$

so that

$$f_1 = A_{11}e^{w_+ t} + A_{12}e^{w_- t} \qquad \text{(A-4)}$$

$$f_2 = A_{21}e^{w_+ t} + A_{22}e^{w_- t} \qquad \text{(A-5)}$$

At t = 0

$$A_{10} = A_{11} + A_{12}$$

$$A_{20} = A_{21} + A_{22}$$

where A_{10} and A_{20} are the initial filling of the traps by the carrier injection pulse. Now one may put equations (A-4) and (A-5) back into (A-1) and (A-2) and by equating

coefficients of like exponential terms, pairing equations and redefining constants to solve for A_{11}, A_{12}, A_{21}, A_{22}.

They can be written

$$A_{11} = \frac{A_{20} - A_{10}(\alpha_-)}{\alpha_+ - \alpha_-} \qquad A_{12} = \frac{A_{20} - A_{10}\alpha_+}{\alpha_- - \alpha_+}$$

$$A_{21} = \frac{A_{10} - A_{20}\delta_-}{\delta_+ - \delta_-} \qquad A_{22} = \frac{A_{10} - A_{20}\delta_+}{\delta_- - \delta_+}$$

where the new terms are given by

$$\alpha_+ = \frac{a_{21}}{w_+ - a_{22}} \qquad \alpha_- = \frac{a_{21}}{w_- - a_{22}}$$

$$\delta_+ = \frac{a_{12}}{w_+ - a_{11}} \qquad \delta_- = \frac{a_{12}}{w_- - a_{11}}$$

As one can see the coefficients on the exponential terms are rather tedious functions of the emission rates of each of the energy states. The total signal measuring the charge state of the trap can thus be written

$$L(t) = f_1 + f_2 = A_{11}e^{w_1 t} + A_{12}e^{w_2 t} + A_{21}e^{w_1 t} + A_{22}e^{w_2 t}$$

The boxcar output signal is thus given by:

$$S(t) = [f_1(t_1) + f_2(t_1)] - [f_1(t_2) + f_2(t_2)]$$

F5 = 1000000
F6 = 100000000
F7 = 1000000
E1 = 0.4
E2 = 0.3
A5 = 1.00258
RMS ERROR:
0.0011727

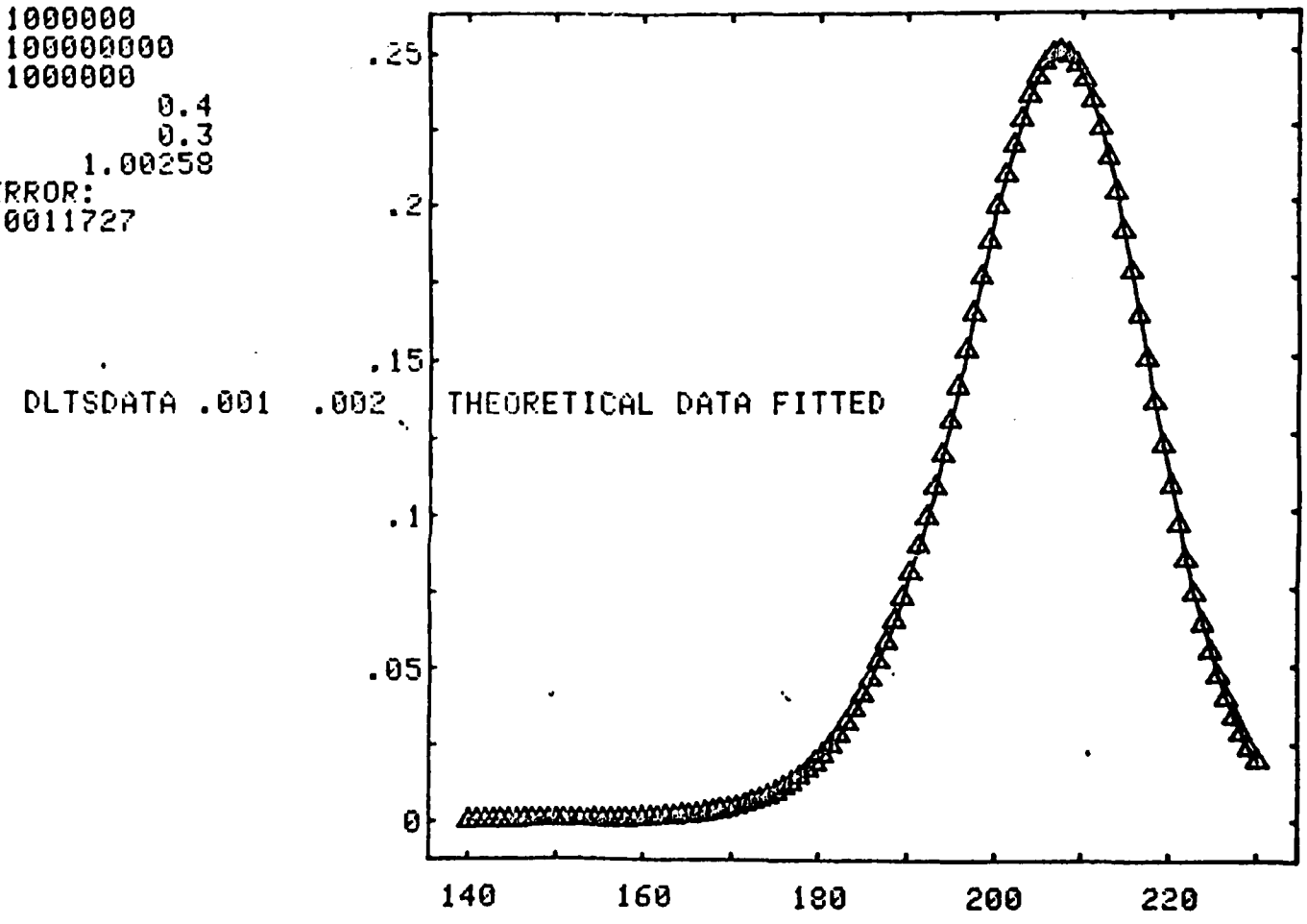


Figure A-1 - Curve Fit on Simulated Ground-Excited State Trap

F5 = 7656910.
F6 = 123577000
F7 = 753707.
E1 = 0.282052
E2 = 0.220704
A5 = 3.91777
RMS ERROR:
0.0271804

BOX1A .00005 .0001

S-214-BA1

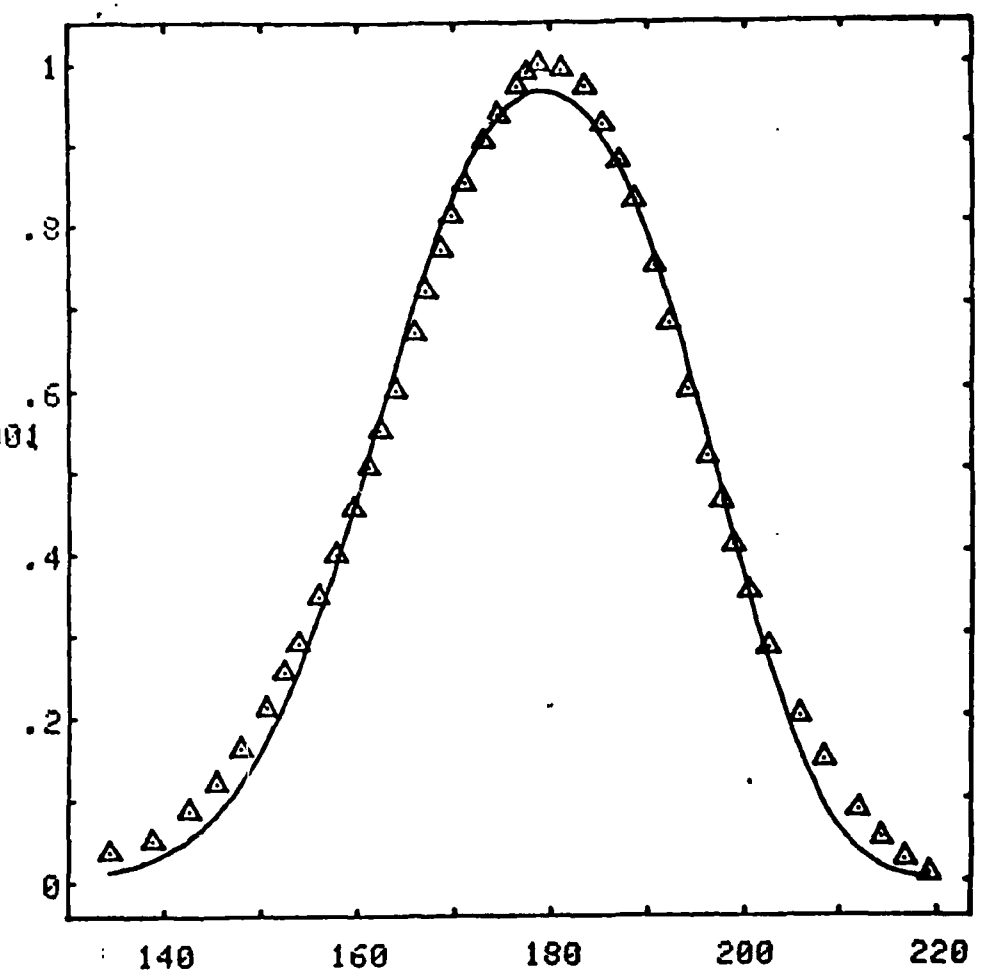


Figure A-2 - Curve Fit on DX Center Data

F5 = 8052600.
F6 = 211748000.
F7 = 921306.
E1 = 0.288544
E2 = 0.211017
A5 = 3.95692
RMS ERROR:
0.0247659

BOX1C .0002 .0004

S-214-BA1

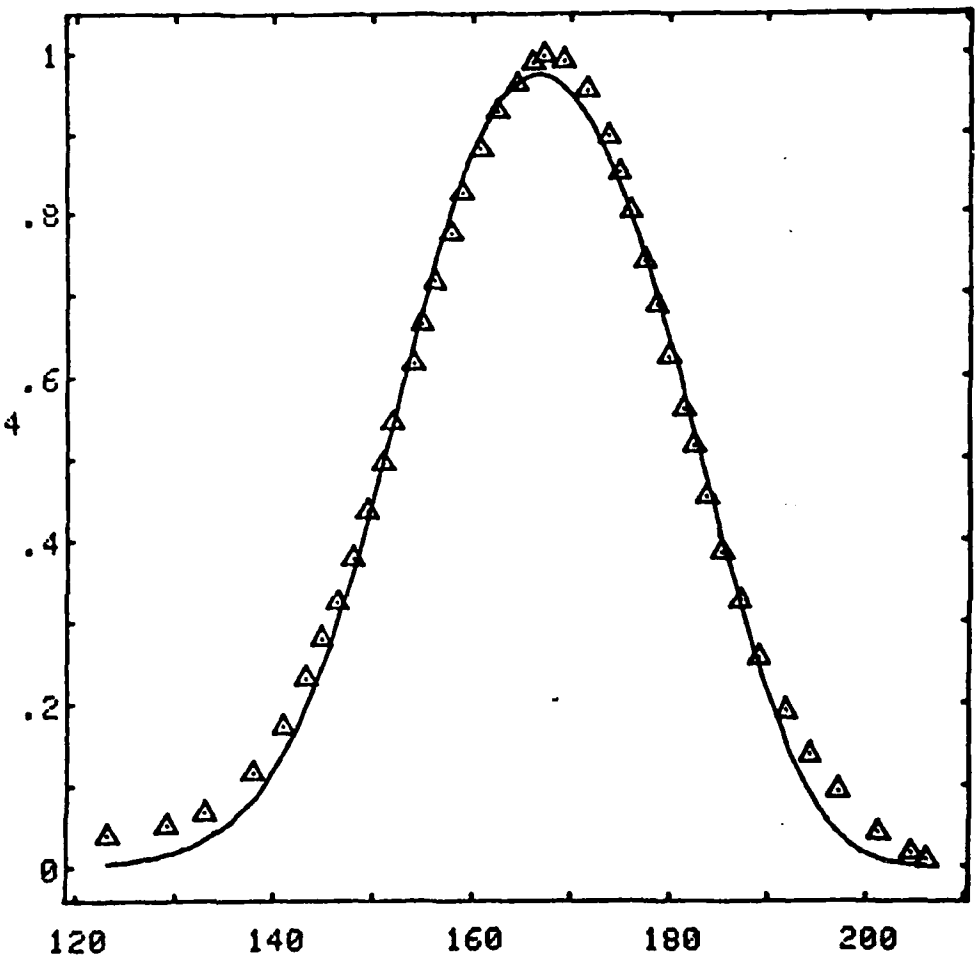


Figure A-3 - Curve Fit on DX Center Data

F5 = 6993090.
F6 = 221607000.
F7 = 957937.
E1 = 0.29118
E2 = 0.192704
A5 = 4.21385
RMS ERROR:
0.0414069

BOX1F .002 .004

S-214-BA1

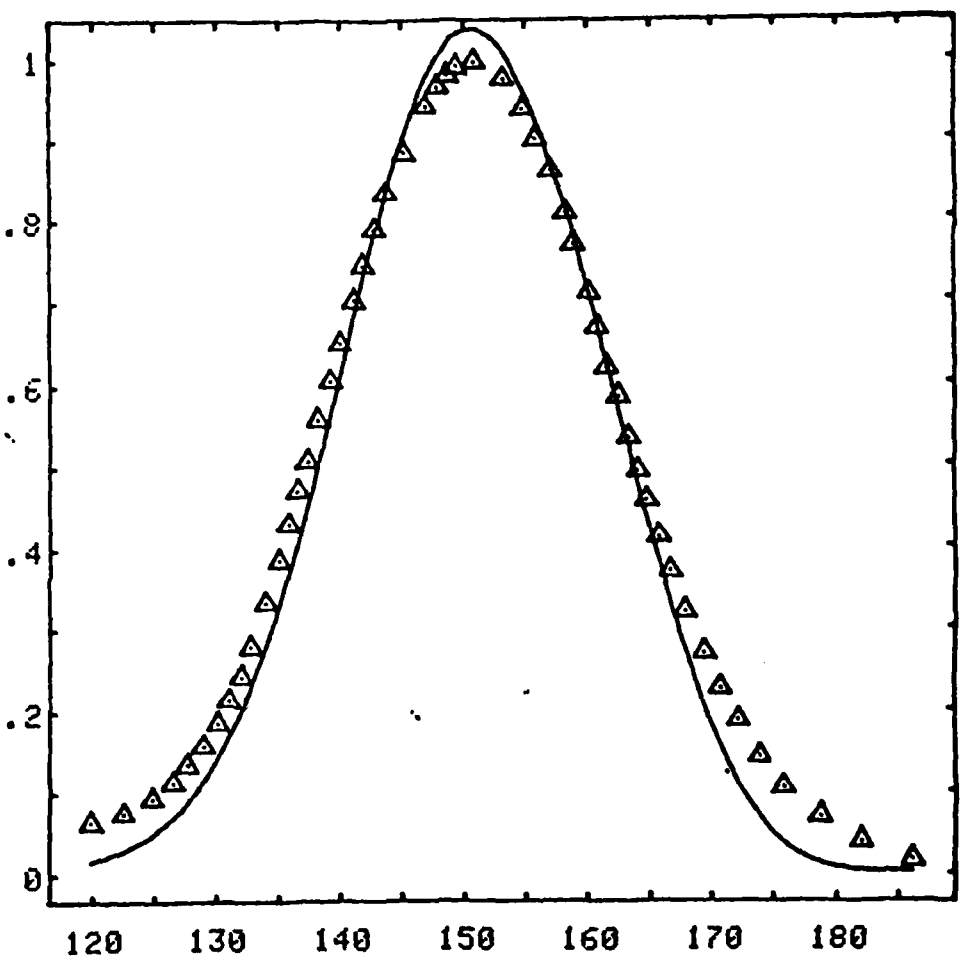


Figure A-4 - Curve Fit on DX Center Data

F5 = 13000000
F6 = 166000000.
F7 = 572000
E1 = 0.29911
E2 = 0.2399
A5 = 3.964
RMS ERROR:
0.0294295

BOX2A .00005,.0001

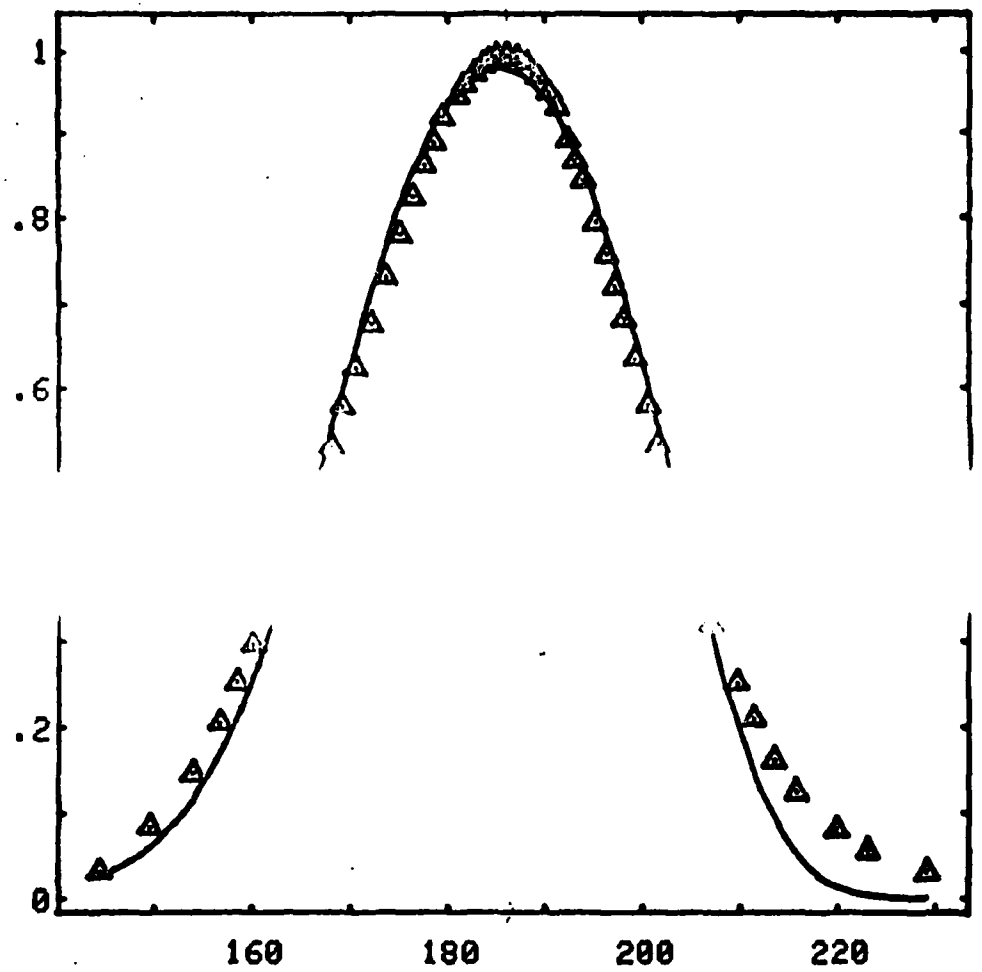


Figure A-5 - Curve Fit on DX Center Data

F5 = 9691930.
F6 = 194765000.
F7 = 362652.
E1 = 0.297655
E2 = 0.237432
A5 = 4.00632
RMS ERROR:
0.0167925

BOX2C .0002 .0004

S-214-BB1

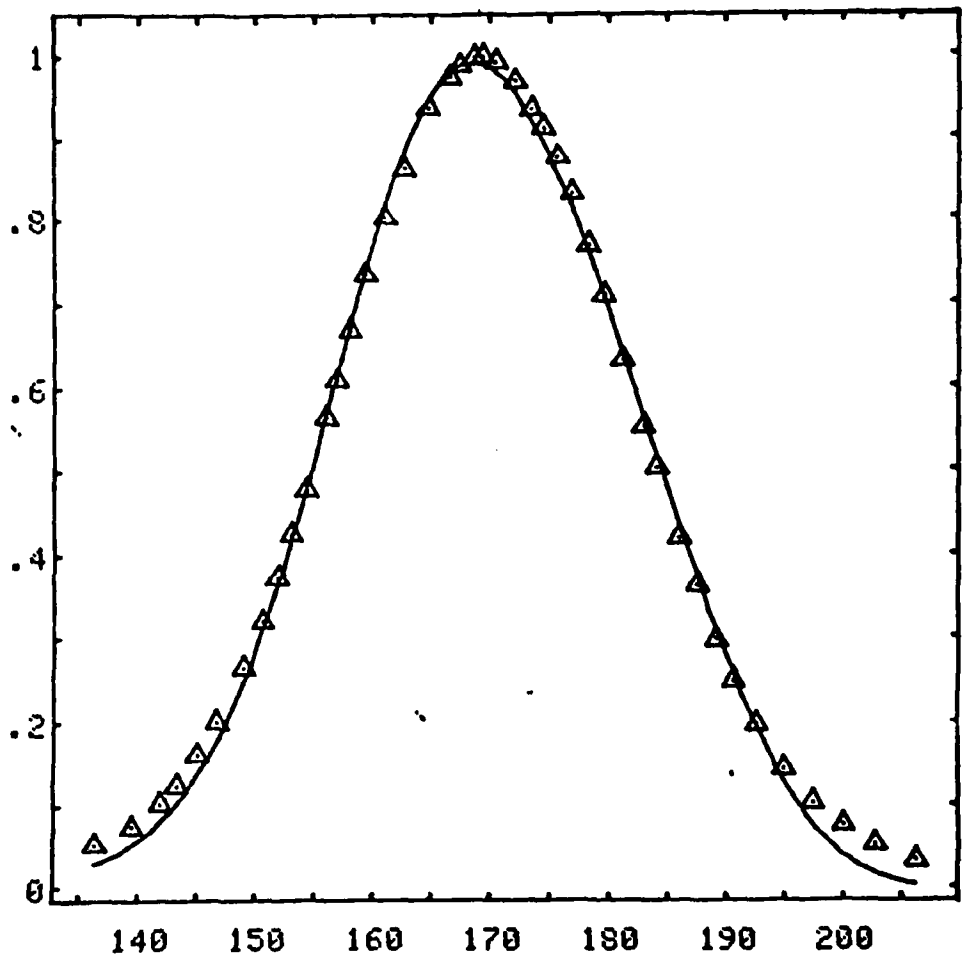


Figure A-6 - Curve Fit on DX Center Data

F5 = 10336600.
F6 = 129329000
F7 = 666614.
E1 = 0.295777
E2 = 0.231951
A5 = 1.9
RMS ERROR:
0.0509389

BOX3A BEST FIT

.00005 .00025

SAMPLE L-107-C1A,1

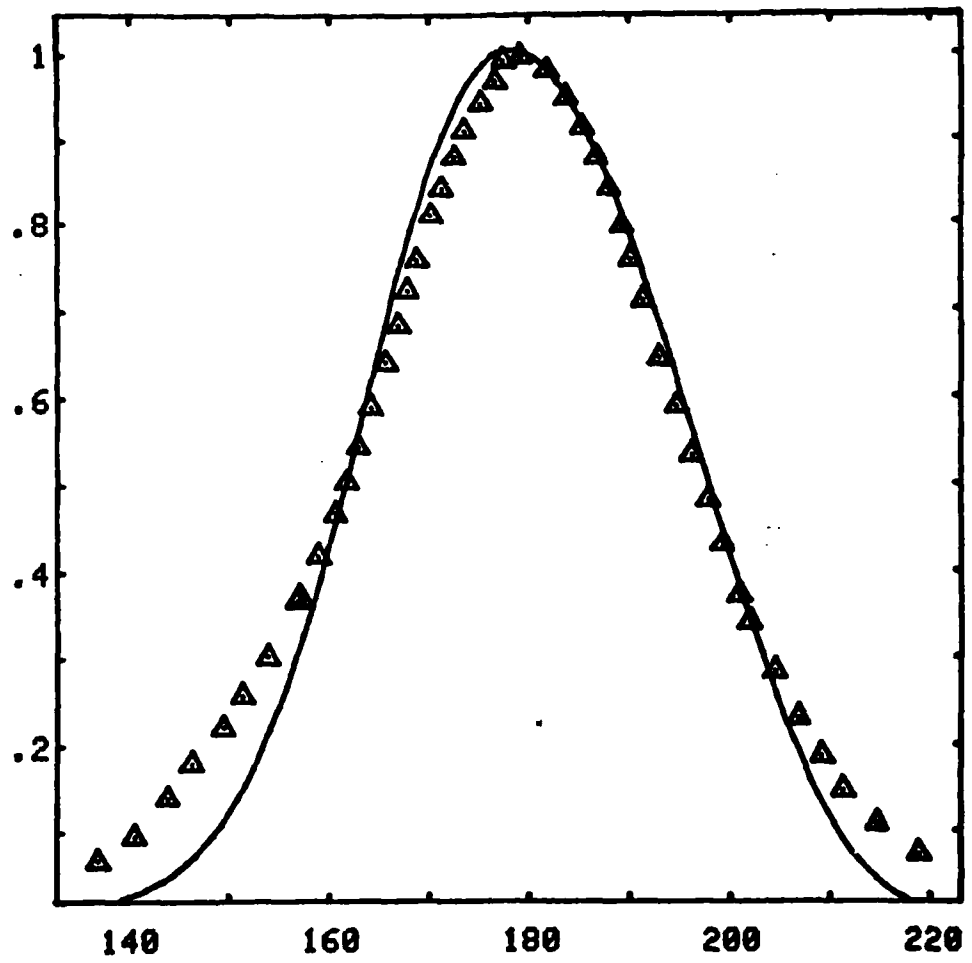


Figure A-7 - Curve Fit on DX Center Data

F5 = 11182200.
F6 = 255694000.
F7 = 366786.
E1 = 0.302514
E2 = 0.234499
A5 = 1.85
RMS ERROR:
0.0453309

BOX3C BEST FIT

.0002 .001

SAMPLE L-107-C1A,1

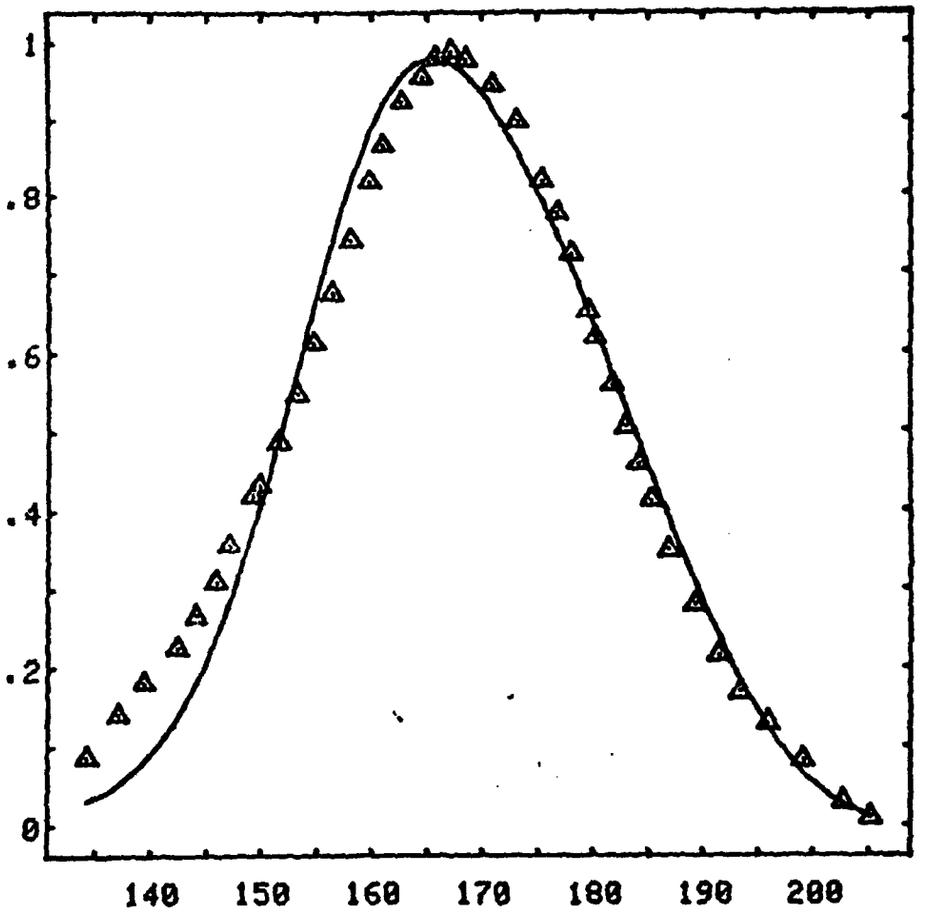


Figure A-8 - Curve Fit on DX Center Data

F5 = 13812600.
F6 = 334922000.
F7 = 206526.
E1 = 0.307938
E2 = 0.224927
A5 = 1.85
RMS ERROR:
0.0332522

BEST FIT BOX3F

.002 .010

L-107-C1A,1

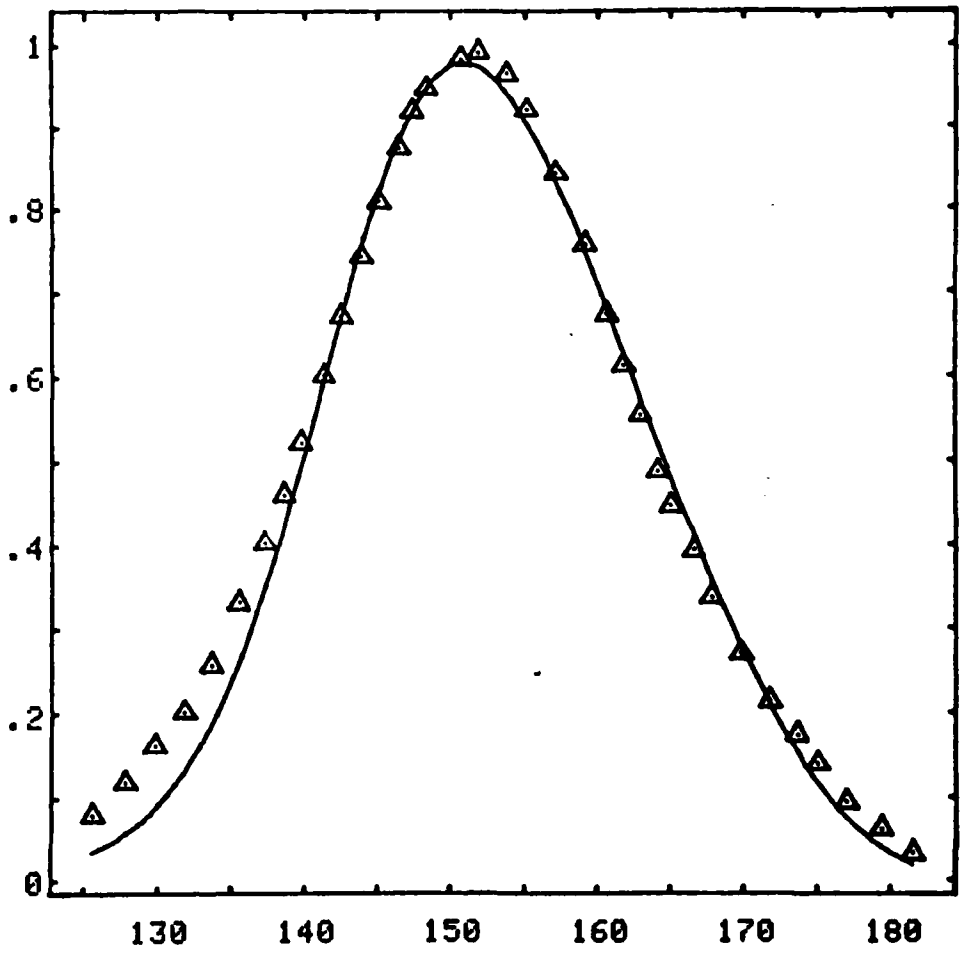


Figure A-9 - Curve Fit on DX Center Data

Index to Computer Programs

Summary of Computer Programs

BILEVEL 1 - Simulates the output of a lock-in amplifier for a trap with two independent energy levels. The initial occupation probabilities must be specified.

BILEVEL 2 - Generates the transient capacitance decay curves that will be analyzed by a lock-in amplifier or boxcar integrator to produce DLTS peaks. The trap is of the two independent state model.

BILEVEL 3 - Simulates a DLTS peak from a lock-in amplifier for a two independent state trap. The initial occupation probabilities are given by thermodynamic equilibrium conditions.

BILEVEL 4 - Generates the transient capacitance decay curves to be analyzed by lock-in amplifier or boxcar integrator for a two independent state trap whose initial occupation probabilities are given by thermodynamic equilibrium conditions.

BOXCAR - Simulates the output of a boxcar integrator based on different initial occupation probabilities of a ground-excited state trap. A DLTS peak is produced.

BOXFIT 1 - A user defined function written in APL for use in the curve fitting program APLLIB***: FITFN. This represents a simple single state trap with fitting parameters A, E, and normalizing parameter A5.

BOXFIT 3 - A user defined function written in APL for use in the curve fitting program APLLIB***: FITFN. This represents a ground-excited state trap with fitting parameters F5, F6, F7, E1, E2, and normalizing parameter A5.

BOXSIN - Generates a DLTS peak from the boxcar integrator based on a simple single state trap.

EXSTATE - Simulates the output of a lock-in amplifier for a trap modeled by a ground-excited state. A DLTS peak results.

EXSTATE 1 - Simulates the output of a lock-in amplifier for a ground-excited state trap in which the initial occupation probabilities of the two levels is changed. Five DLTS peaks are generated.

EXSTATE 2 - Simulates the output of the lock-in amplifier for a ground-excited state trap in which the initial occupation probabilities are determined by thermodynamic equilibrium conditions.

EXSTBOX - Simulates the output of a boxcar integrator for a ground-excited state trap with thermodynamic equilibrium conditions. This generates one data peak.

OMEGA - Prints out the inverse time constants (w_1 and w_2) for the exponential terms in the solution of the coupled emission rate equations for the ground-excited state trap model. Generates values for twenty degrees at intervals of ten degrees.

TRIXFIT - Performs a least-squares fit on a data file containing a digitzed DLTS peak. The fit function represents the output of a lock-in amplifier for a simple single state trap. The program creates a matrix of fits based on initial parameter inputs, picking out the best combination of parameters for a graphics display of the fit.

Note: All programs written in BASIC with the exception of BOXFIT 1 and BOXFIT 3 which are written in APL.

BILEVEL1

```
100 REM    THIS IS A PROGRAM THAT SIMULATES THE OUTPUT OF A
110 REM  LOCK-IN AMPLIFIER FOR A DLTS RUN ON A TWO LEVEL TRAP
120 REM  WITHIN THE BAND GAP.  THE SYSTEM CONSISTS OF TWO INDE-
130 REM  PENDENT, COMMUNICATING ENERGY STATES AT E1 AND E2.
140 REM  THE RESULTING DATA IS A PLOT OF THE FOURIER TRANSFORMED
150 REM  TRANSIENT CAPACITANCE SIGNAL VS. TEMP.
155 REM  THE USER MUST SPECIFY THE INITIAL OCCUPATION
157 REM  PROBABILITIES OF THE TRAP.
160 K=8.618E-5
170 PRINT "RESULTS FILENAME?"
180 INPUT A$
190 FILE#1:A$
200 PRINT "SCRATCH"; ;A$;"?"
210 INPUT B$
220 IF B$="NO" THEN 240
230 SCRATCH #1
240 PRINT "INPUT PREFACTOR VALUES:A1C,A2C,A12,A21"
250 INPUT F5,F6,F7,F8
260 PRINT "INPUT ENERGIES--E1,E2"
270 INPUT E1,E2
280 PRINT  INPUT LOCK-IN FREQ."
290 INPUT F
300 F=1/F
310 PRINT "INPUT # OF INTEGRATIONS"
320 INPUT H
330 M=F/H
340 PRINT "TEMP. RANGE?"
350 INPUT T1,T2
360 Q=(T2-T1)/100
370 FOR G=0 TO 100
380 A=B=0
390 T=T1+G*Q
400 N3=N4=1000
410 N1=N2=1000
420 D1=D2=D3=D4=S=A=B=0
430 A1=F5*T^2*EXP(-E1/(K*T))
440 A2=F6*T^2*EXP(-E2/(K*T))
450 A3=F7*EXP(-(E1-E2)/(K*T))
460 A4=F7
470 FOR I=0 TO H
480 T5=I*M
490 D=N3-N1
500 J=N4-N2
510 D1=(-A1*N1+A4*N2*(D)-A3*N1* J))*M
520 D2=(-A2*N2+A3*N1*(J)-A4*N2*(D))*M
```

BILEVEL1 (CONT'ED)

```
530 N1=N1+D1
540 N2=N2+D2
550 S=N1+N2
560 IF S<1E-10 THEN 620
570 D3=(S*COS(2*3.142*(T5/F)))*M
580 D4=(S*SIN(2*3.142*(T5/F)))*M
590 A=A+D3
600 B=B+D4
610 NEXT I
620 A=A*2/F
630 B=B*2/F
640 L=2/(3.142)*(A*SIN(P)+B*COS(P))
650 PRINT#1:T,L
660 PRINT T;L
670 NEXT G
680 PRINT#1:"1E37","1E37"
690 PRINT "DONE"
700 PRINT "ANOTHER RUN?"
710 INPUT A$
720 IF A$="YES" THEN 740
730 GO TO 750
740 GO TO 240
750 END
```

BILEVEL2

```
100 REM  THIS IS A NUMERICAL INTEGRATION PROGRAM GENERATING THE
110 REM  ACTUAL TRANSIENT CAPACITANCE CURVES FOR A TWO LEVEL
120 REM  SYSTEM WITHIN THE VALENCE-CONDUCTION BAND ENERGY GAP.
140 REM  ELEVEN CURVES ARE GENERATED BETWEEN TWO SPECIFIED TEMPS.
150 REM  SHOWING THE CHANGE IN TRAP EMPTYING WITH INCREASING TEMP.
160 REM  THESE CURVES ARE MULTIPLIED BY THE FIRST FOURIER COMPONENT
170 REM  AND NUMERICALLY INTEGRATED IN "BILEVEL1" TO CREATE A DLTS
180 REM  PEAK REFLECTING THE GIVEN PARAMETERS.  THE INITIAL OCCUPA-
190 REM  TION LEVELS OF EACH TRAP MUST BE SPECIFIED BY THE USER.
200 K=8.618E-5
210 PRINT "RESULTS FILENAME?"
220 INPUT A$
230 FILE#1:A$
240 PRINT "SCRATCH"; ;A$;"?"
250 INPUT B$
260 IF B$="NO" THEN 280
270 SCRATCH #1
280 F5=2.6E4
290 PRINT "INPUT A2"
300 INPUT F6
310F7=F8=.376
320 E1=.25
330 E2=.3
340 PRINT "INPUT LOCK-IN FREQ."
350 INPUT F
360 F=1/F
370 PRINT "INPUT # OF INTEGRATIONS"
380 INPUT H
390 M=F/H
400 PRINT "TEMP. RANGE?"
410 INPUT T1,T2
420 Q=(T2-T1)/10
430 FOR G=0 TO 10
440 T=T1+G*Q
450 N3=N4=1000
460 N1=N2=1000
470 D1=D2=D3=D4=S=A=B=0
480 A1=F5*T^2*EXP(-E1/(K*T))
490 A2=F6*T^2*EXP(-E2/(K*T))
500 A3=F7*EXP(-(E1-E2)/(K*T))
510 A4=F7
520 FOR I=0 TO H
530 T5=I*M
540 D=N3-N1
550 J=N4-N2
```

BILEVEL2 (CONT'ED)

```
560 D1=(-A1*N1+A4*N2*(D)-A3*N1*(J))*M
570 D2=(-A2*N2+A3*N1*(J)-A4*N2*(D))*M
580 N1=N1+D1
590 N2=N2+D2
600 S=N1+N2
610 IF S<1E-3 THEN 660
620 IF INT(I/10)=I/10 THEN 640
630 GO TO 650
640 PRINT#1:T5,S
650 NEXT I
660 PRINT#1:"1E37","1E37"
670 NEXT G
680 PRINT "DONE"
690 PRINT "ANOTHER TEMP. RANGE?"
700 INPUT A$
710 IF A$="YES" THEN 730
720 GO TO 740
730 GO TO 400
740 END
```

BILEVEL3

```
100 REM    THIS IS A PROGRAM THAT GENERATES A DLTS PEAK
105 REM FOR A TWO LEVEL TRAP WITHIN THE SEMICONDUCTOR
110 REM ENERGY GAP.  THIS EXPERIMENTAL SYSTEM USES A LOCK-IN
120 REM AMPLIFIER FOR SIGNAL ANALYSIS.
170 K=8.618E-5
180 PRINT "RESULTS FILENAME?"
190 INPUT A$
200 FILE#1:A$
210 PRINT "SCRATCH"; ;A$;"?"
220 INPUT B$
230 IF B$="NO" THEN 250
240 SCRATCH #1
250 PRINT "INPUT PREFACTOR VALUES:A1C,A2C"
260 INPUT F5,F6
270 PRINT "INPUT ENERGIES--E1,E2"
280 INPUT E1,E2
290 PRINT "INPUT LOCK-IN FREQ."
300 INPUT F
310 F=1/F
320 PRINT "INPUT # OF INTEGRATIONS"
330 INPUT H
340 M=F/H
350 PRINT "INPUT # OF TRAPS"
360 INPUT N
370 PRINT "INPUT A12"
380 INPUT F7
390 PRINT "TEMP RANGE?"
400 INPUT T1,T2
410 Q=(T2-T1)/25
420 FOR G=0 TO 25
430 A=B=0
440 T=T1 G*Q
450 N3=N4=1000
460 N1=N2=1000
470 D1=D2=D3=D4=S=A=B=0
480 F1=1/(1+EXP(-(E1-E2)/(K*T)))
490 F2=1-F1
500 A1=F5*T^2*EXP(-E1/(K*T))
510 A2=F6*T^2*EXP(-E2/(K*T))
520 A3=F7*EXP(-(E1-E2)/(K*T))
530 A4=F7
540 FOR I=0 TO H
550 T5=I*M
560 D1=((A4*F2)-(A3*F1)-(A1*F1))*M
570 D2=((A3*F1)-(A4*F2)-(A2*F2))*M
```

BILEVEL3 (CONT'ED)

```
580 F1=F1+D1
590 F2=F2+D2
600 N1=F1*N
610 N2=F2*N
620 S=N1+N2
630 IF S<1E-36 THEN 690
640 D3=(S*COS(2*3.142*(T5/F)))*M
650 D4=(S*SIN(2*3.142*(T5/F)))*M
660 A=A+D3
670 B=B+D4
680 NEXT I
690 A=A*2/F
700 B=B*2/F
710 L=2/(3.142)*(A*SIN(P)+B*COS(P))
720 PRINT#1:T,L
730 PRINT T;L
740 NEXT G
750 PRINT#1:"1E37" "1E37"
760 PRINT "DONE"
770 END
```

BILEVEL4

```
100 REM    THIS PROGRAM GENERATES THE TRANSIENT CAPACITANCE
105 REM  CURVES FOR A TWO INDEPENDENT ENERGY LEVEL SYSTEM WITHIN
110 REM  THE BABD GAP.  THE INITIAL OCCUPATION PROBABILITIES
115 REM  ARE SET BY THERMODYNAMIC EQUILIBRIUM CONDITIONS.
120 REM  TWENTY CURVES ARE GENERATED SHOWING THE CHANGE IN
125 REM  TRANSIENT CAPACITANCE WITH INCREASING TEMPERATURE.
130 REM  THE X-AXIS IS TIME.
160 K=8.618E-5
170 PRINT "RESULTS FILENAME?"
180 INPUT A$
190 FILE#1:A$
200 PRINT "SCRATCH"; ;A$;"?"
210 INPUT B$
220 IF B$="NO" THEN 240
230 SCRATCH #1
240 F5=2.6E4
250 F6=6.08E6
260 PRINT "INPUT A12"
270 INPUT F7
280 E1=.6
290 e2=.3
300 PRINT "INPUT LOCK-IN FREQ."
310 INPUT F
320 F=1/F
330 H=5000
340 M=F/H
350 PRINT "TEMP. RANGE?"
360 INPUT T1,T2
370 N=1000
380 Q=(T2-T1)/20
390 FOR G=0 TO 20
400 A=B=0
410 T=T1+G*Q
420 N3=N4=1000
430 N1=N2=1000
440 D1=D2=D3=D4=S=A=B=0
450 F1=1/(1+EXP(-(E1-E2)/(K*T)))
460 F2=1-F1
470 A1=F5*T^2*EXP(-E1/(K*T))
480 A2=F6*T^2*EXP(-E2/(K*T))
490 A3=F7*EXP(-(E1-E2)/(K*T))
500 A4=F7
510 FOR I=0 TO H
520 T5=I*M
530 D1=((A4*F2)-(A3*F1)-(A1*F1))*M
```

BILEVEL4 (CONT'ED)

```
540 D2=((A3*F1)-(A4*F2)-(A2*F2))*M
550 F1=F1+D1
560 F2=F2+D2
570 N1=F1*N
580 N2=F2*N
590 S=N1+N2
600 IF S<1E-25 THEN 650
610 IF INT(I/20)=I/20 THEN 630
620 GO TO 640
630 PRINT#1:T5,S
640 NEXT I
650 PRINT#1:"1E37","1E37"
660 NEXT G
670 PRINT#1:"1E37","1E37"
680 PRINT "DONE"
690 PRINT "ANOTHER RUN?"
700 INPUT A$
710 IF A$="YES" THEN 730
720 GO TO 740
730 GO TO 240
740 END
```

BOXCAR

```
100 REM    THIS PROGRAM SIMULATES THE OUTPUT OF A BOXCAR
110 REM  INTEGRATOR, CREATING A FILE WITH DIGITIZED CURVES
120 REM  REPRESENTING DLTS PEAKS BASED ON DIFFERENT INITIAL
130 REM  FILLINGS OF A GROUND-EXCITED STATE MODEL OF AN ELEC-
140 REM  TRON TRAP.
150 DATA 1,0,.75,.25,.5,.5,.25,.75,0,1,100,100
160 K=8.625E-5
170 PRINT "INPUT PREFACTORS A1C,A2C,A12"
180 INPUT F5,F6,F7
190 PRINT "RESULTS FILENAME?"
200 INPUT A$
210 FILE#1:A$
220 PRINT "SCRATCH";"  ";A$
230 INPUT B$
240 IF B$="NO" THEN 270
250 SCRATCH #1
260 PRINT A$;"  ";"SCRATCHED"
270 PRINT "INPUT E1,E2"
280 INPUT E1,E2
290 PRINT "LOCK-IN FREQ.?"
300 INPUT F
310 F=1/F
320 PRINT "INPUT SAMPLING TIME FRACTIONS (0-1)"
330 INPUT Z,Z1
340 S1=Z*F
350 S2=Z1*F
360 PRINT "NUMBER OF DATA POINTS?"
370 INPUT H
380 M=F/H
390 PRINT "TEMPERATURE RANGE?"
400 INPUT T1,T2
410 Q=(T2-T1)/100
420 READ H2,H1
430 FOR I=0 TO 100
440 A=E=D3=D4=0
450 T=T1+Q*I
460 A0=H2
470 B0=H1
480 IF H2>1 THEN 910
490 R1=F5*T^2*EXP(-E1/(K*T))
500 R2=F6*T^2*EXP(-E2/(K*T))
510 R3=F7*EXP(-(E1-E2)/(K*T))
520 R4=f7
530 B=-(R1+R2+R3+R4)
540 D=(R2+R4-R1-R3)^2+4*R3*R4
```

BOXCAR (CONT'ED)

```
550 C=SQR(D)
560 W1=(B+C)/2
570 W2=(B-C)/2
580 B1=-(R1+R3)
590 B2=R3
600 B3=R4
610 B4=-(R2+R4)
620 C1=B2/(W1-B4)
630 C2=B2/(W2-B4)
640 C3=B3/(W1-B1)
650 C4=B3/(W2-B1)
660 A1=(B0-(A0*C2))/(C1-C2)
670 A2=(B0-(A0*C1))/(C2-C1)
680 A3=(A0-(B0*C4))/(C3-C2)
690 A4=(A0-(B0*C3))/(C4-C3)
700 FOR G=0 TO H
710 T5=G*M
720 IF W2*T5<-40 THEN 760
730 F1=A1*EXP(W1*T5)+A2*EXP(W2*T5)
740 F2=A3*EXP(W1*T5)+A4*EXP(W2*T5)
750 GO TO 780
760 F1=A1*EXP(W1*T5)
770 F2=A3*EXP(W1*T5)
780 S=F1+F2
790 IF T5=S1 THEN 820
800 IF T5=S2 THEN 840
810 GO TO 870
820 L1=S
830 GO TO 870
840 L2=S
850 L=(L1-L2)/1000
860 PRINT#1:T,L
870 NEXT G
880 NEXT I
890 PRINT#1:1E37,1E37
900 GO TO 420
910 END
```

BOXFIT1

```
.CM   THIS FUNCTION IS A USER DEFINED FUNCTION IN APL USED
.CM IN THE FITTING PROGRAM APLLIB***:FITFN TO FIT DATA TO
.CM THE OUTPUT OF A BOXCAR INTEGRATOR DOING A DLTS
.CM RUN ON A SIMPLE SINGLE STATE ELECTRON TRAP.
$ Z=TIME EF X
[1]   R=A#(X*2)#(*(-E%(8.617E"5#X)))
[2]   Z=*(-TIME#R)
$K
$ Z=SIG X
[1]   Z=(TIMF' EF X)-TIME2 EF X
[2]   Z=A5#Z
$
```

BOXFIT3

```
.CM    THIS PROGRAM IS A USER DEFINED FUNCTION IN APL USED
.CM  IN THE FITTING PROGRAM APLLIB***:FITFN.  THE FUNCTION
.CM  CREATES THE OUTPUT OF A BOXCAR INTEGRATOP ON A DLTS
.CM  SWEEP OF A SAMPLE CONTAINING ELECTRON TRAPS OF THE
.CM  COMMUNICATING GROUND-EXCITED STATE MODEL.  THE DATA
.CM  FILE MUST BE IN THE FORM OF X-Y PAIRS: TEMPERATURE AND
.CM  SIGNAL.
$   VV=M CHECK V
[1] LV=M>.ABV
[2] VV=(LV#V)+M#(#V)#.NTLV
$K
A10=         0.98
A20=         0.02
$   Z= SIG X
[1]  R1=F5#(X*2)#*-(50 CHECK E1%(X#8.617E"5))
[2]  R2=F6#(X*2)#*-(50 CHECK E2%(X#8.617E"5))
[3]  R3=F7#*-(50 CHECK (E1-E2)%(X#8.617E"5))
[4]  B=-(R1+R2+R3+F7)
[5]  D=(((R2+F7-R1+R3)*2)+4#R3#F7)*0.5
[7]  C3=F7%(((B+D)%2)+(R1+R3))
[9] A4=(A10-(A20#C3))#(((B-D)%2)+R1+R3)#(((B+D)%2)+R1+R3)%(D#F7)
[10] W1=(B+D)%2 ;W2=(B-D)%2;
[11] W11=W1#TIME1 ;W12=W1#TIME2;
[12] W21=W2#TIME1 ;W22=W2#TIME2;
[13] W11=50 CHECK W11 ;W12=50 CHECK W12;
[14] W21=50 CHECK W21 ;W22=50 CHECK W22;
[15] Z=(C3+1)#(A20-A4)#(*W11)-*W12
[16] Z=Z+(A10+A4-C3#(A20-A4))#(*W21)-*W22
[17] Z=Z#A5
$K
```

BOXSIN

```
100 REM    THIS PROGRAM CREATES A BOXCAR INTEGRATOR DLTS
110 REM  PEAK BASED ON A SIMPLE SINGLE STATE ELECTRON TRAP.
120 PRINT "SAVE RESULTS(YES/NO)"
130 INPUT A$
140 IF A$="NO" THEN 240
150 PRINT "STORAGE FILENAME?"
160 INPUT B$
170 FILE#1: B$
180 PRINT "EMPTY FILE";B$;"?"
190 INPUT C$
200 IF C$="NO" THEN 230
210 SCRATCH #1
220 GO TO 240
230 PRINT #1:1E37,1E37
240 PRINT "ENERGY GAP (EV)?"
250 INPUT E
260 PRINT "TEMP. BOUNDARIES (K)?"
270 INPUT L,H
280 PRINT "INPUT T1,T2 IN MILLISEC"
290 INPUT T6,T7
300 T6=T6/1000
310 T7=T7/1000
320 PRINT "INPUT PREFACTOR A"
330 INPUT F
340 K=8.617E-5
350 PRINT "INPUT NORMALIZATION"
360 INPUT N
370 Q=(H-L)/100
380 FOR I=0 TO 100
390 T=L+Q*I
400 R=F*(T^2)*EXP(-E/(K*T))
410 S=EXP(-R*T6)-EXP(-R*T7)
420 S=S*N
430 IF A$="NO" THEN 450
440 PRINT#1:T,S
450 NEXT I
460 PRINT "DONE"
470 END
```

EXSTATE

```
100 REM    THIS PROGRAM GENERATES THE THEORETICAL OUTPUT OF A
110 REM  LOCK-IN AMPLIFIER USED IN A DLTS RUN ON A TRAP MODELED
120 REM  BY A COMMUNICATING GROUND-EXCITED STATE SYSTEM.  PARA-
130 REM  METERS MAY BE ADJUSTED IN ORDER TO VIEW THE EFFECT ON
140 REM  THE OUTPUT.
150 Z9=0
160 K=8.617E-5
170 PRINT  INPUT PREFACTORS A1C.A2C,A12
180 INPUT F5,F6,F7
190 PRINT "RESULTS FILENAME?
200 INPUT A$
210 FILE#1:A$
220 PRINT "SCRATCH ;"    ;A$
230 INPUT B$
240 IF B$= NO  THEN 161
250 SCRATCH #1
260 PRINT A$;"    ; SCRATCHED
270 PRINT  INPUT E1,E2
280 INPUT E1,E2
290 PRINT "LOCK-IN FREQ ?
300 INPUT F
310 F=1/F
320 PRINT "NUMBER OF DATA POINTS?
330 INPUT H
340 M=F/H
350 PRINT "TEMPERATURE RANGE?
360 INPUT T1.T2
370 Q=(T2-T1)/H
380 FOR I=0 TO H
390 A=E=D3=D4=0
400 T=T1+Q*I
410 A0=1/(1+EXP(-(E1-E2)/(K*T)))
420 B0=1-A0
430 R1=F5*T 2*EXP(-E1/(K*T))
440 R2=F6*T 2*EXP(-E2/(K*T))
450 R3=F7*EXP(-(E1-E2)/(K*T))
460 R4=F7
470 B=-(R1+R2+R3+R4)
480 D=(R2+R4-R1-R3) 2+4*R3*R4
490 C=SQR(D)
500 W1=(B+C)/2
510 W2=(B-C)/2
520 B1=-(R1+R3)
530 B2=R3
540 B3=R4
```

EXSTATE (CONT'ED)

```
550 B4=-(R2+R4)
560 C1=B2/(W1-B4)
570 C2=B2/(W2-B4)
580 C3=B3/(W1-B1)
590 C4=B3/(W2-B1)
600 A1=(B0-(A0*C2))/(C1-C2)
610 A2=(B0-(A0*C1))/(C2-C1)
620 A3=(A0-(B0*C4))/(C3-C2)
630 A4=(A0-(B0*C3))/(C4-C3)
640 FOR G=0 TO H
650 T5=G*M
660 IF w2*T5<-40 THEN 591
670 F1=A1*EXP(W1*T5)+A2*EXP(W2*T5)
680 F2=A3*EXP(W1*T5)+A4*EXP(W2*T5)
690 GO TO 621
700 IF W1*T5<-40 THEN 621
710 F1=A1*EXP(W1*T5)
720 F2=A3*EXP(W1*T5)
730 S=F1+F2
740 IF S<1E-25 THEN 681
750 D3=(S*COS(2*3.142*(T5/F)))*M
760 D4=(S*SIN(2*3.142*(T5/F)))*M
770 A=A+D3
780 E=E+D4
790 NEXT G
800 A=A*2/F
810 E=E*2/F
820 L=2/(3.142)*(A*SIN(P)+E*COS(P))
830 PRINT#1:T,L
840 IF Z9>0 THEN 791
850 IF L<L1 THEN 771
860 L1=L
870 GO TO 791
880 PRINT "T MAX= ;T
890 Z9=T
900 NEXT I
910 PRINT#1:"1E37 , 1E37
920 PRINT "DONE"
930 END
```

EXSTATE1

```
10 REM    THIS PROGRAM GENERATES LOCK-IN AMPLIFIER
20 REM  DLTS PEAKS BASED ON INPUTS BY THE USER.  FIVE
30 REM  PEAKS ARE GENERATED REFLECTING THE CHANGE IN
40 REM  LINESHAPE OF DIFFERENT INITIAL OCCUPATION
50 REM  PROBABILITIES OF THE GROUND AND EXCITED STATES
60 REM  USED IN THIS MODEL.  THE FILLING PROBABILITIES
65 REM  ARE LISTED IN THE DATA STATEMENT.
100 DATA 1,0,.75,.25,.5, 5,.25,.75,.0,1,100,100
110 K=8.625E-5
120 PRINT  INPUT PREFACTORS A1C,A2C,A12
130 INPUT F5,F6,F7
140 PRINT "RESULTS FILENAME?
150 INPUT A$
160 FILE#1:A$
170 PRINT  SCRATCH ';"    ;A$
180 INPUT B$
190 IF B$= NO  THEN 220
200 SCRATCH #1
210 PRINT A$;"    ;"SCRATCHED
220 PRINT "INPUT E1,E2"
230 INPUT E1,E2
240 PRINT  LOCK-IN FREQ ?
250 INPUT F
260 F=1/F
270 PRINT  NUMBER OF DATA POINTS?
280 INPUT H
290 M=F/H
300 PRINT "TEMPERATURE RANGE?
310 INPUT T1,T2
320 Q=(T2-T1)/100
330 READ H2,H1
340 FOR I=0 TO H
350 A=E=D3=D4=0
360 T=T1+Q*I
370 A0=H2
380 B0=H1
390 IF H2>1 THEN 840
400 R1=F5*T 2*EXP(-E1/(K*T))
410 R2=F6*T 2*EXP(-E2/(K*T))
420 R3=F7*EXP(-(E1-E2)/(K*T))
430 R4=f7
440 B=-(R1+R2+R3+R4)
450 D=(R2+R4-R1-R3) 2+4*R3*R4
460 C=SQR(D)
470 W1=(B+C)/2
```

AD-A109 701 NAVAL ACADEMY ANNAPOLIS MD F/G 20/12
CHARACTERIZATION OF TRAPPING STATES IN SEMICONDUCTORS.(U)
JUN 81 H S HOPKINS
UNCLASSIFIED USNA-TSPR-111 NL

END
DATE FILMED
02-82
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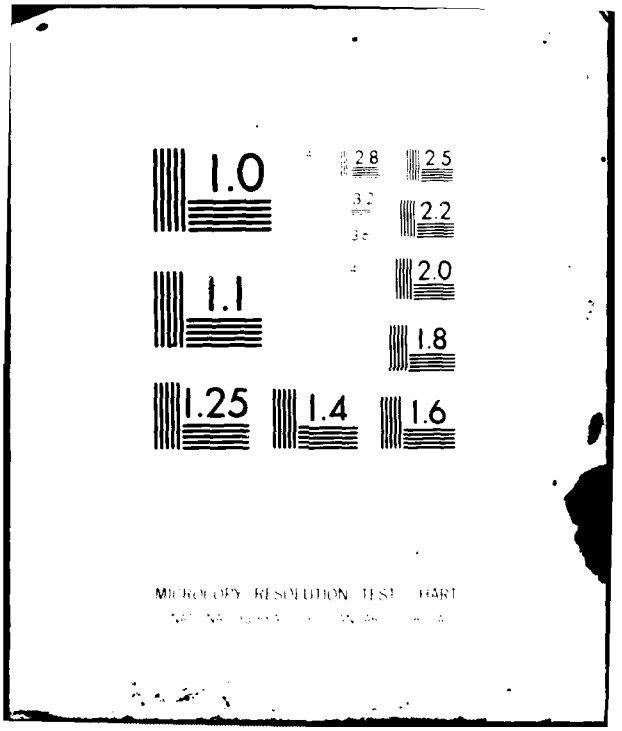
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2.8
2.5
3.2
2.2
3.6
4
2.0
1.1
1.8
1.25
1.4
1.6
MICROCOPY RESOLUTION TEST CHART

EXSTATE1 (CONT'ED)

```
480 W2=(B-C)/2
490 B1=-(R1+R3)
500 B2=R3
510 B3=R4
520 B4=-(R2+R4)
530 C1=B2/(W1-B4)
540 C2=B2/(W2-B4)
550 C3=B3/(W1-B1)
560 C4=B3/(W2-B1)
570 A1=(B0-(A0*C2))/(C1-C2)
580 A2=(B0-(A0*C1))/(C2-C1)
590 A3=(A0-(B0*C4))/(C3-C2)
600 A4=(A0-(B0*C3))/(C4-C3)
610 FOR G=0 TO H
620 T5=G*M
630 IF W2*T5<-40 THEN 670
640 F1=A1*EXP(W1*T5)+A2*EXP(W2*T5)
650 F2=A3*EXP(W1*T5)+A4*EXP(W2*T5)
660 GO TO 690
670 F1=A1*EXP(W1*T5)
680 F2=A3*EXP(W1*T5)
690 S=F1+F2
700 IF S<1E-25 THEN 750
710 D3=(S*COS(2*3.142*(T5/F)))*M
720 D4=(S*SIN(2*3 142*(T5/F)))*M
730 A=A+D3
740 E=E+D4
750 NEXT G
760 A=A*2/F
770 E=E*2/F
780 L=2/(3.142)*(A*SIN(P)+E*COS(P))
790 PRINT#1:T,L
800 NEXT I
810 PRINT#1:"1E37 , 1E37
820 PRINT "DONE"
830 GO TO 330
840 END
```

EXSTATE2

```
10    THIS PROGRAM GENERATES A LOCK-IN PLTS PEAK
20  BASED ON THE THERMODYNAMIC INITIAL FILLING OF
30  THE GROUND AND EXCITED STATE.
100 K=8.625E-5
110 PRINT "INPUT PREFACTORS A1G,A2G,A12"
120 INPUT F5,F6,F7
130 PRINT "RESULTS FILENAME?"
140 INPUT A$
150 FILE#1:A$
160 PRINT "SCRATCH";"  ";A$
170 INPUT B$
180 IF B$="NO" THEN 120
190 SCRATCH #1
200 PRINT A$;"  ";"SCRATCHED"
210 PRINT "INPUT E1,E2"
220 INPUT E1,E2
230 PRINT "LOCK-IN FREQ.?"
240 INPUT F
250 P=1/F
260 PRINT "NUMBER OF DATA POINTS?"
270 INPUT H
280 M=F/H
290 PRINT "TEMPERATURE RANGE?"
300 INPUT T1,T2
310 G=(T2-T1)/100
320 FOR I=0 TO 100
330 A=B=B3=B4=0
340 T=T1+G*I
350 A0=1/(1+EXP(-(E1-E2)/(K*T)))
360 B0=1-A0
370 R1=F5*T^2*EXP(-E1/(K*T))
380 R2=F6*T^2*EXP(-E2/(K*T))
390 R3=F7*EXP(-(E1-E2)/(K*T))
400 R4=F7
410 B=-(R1+R2+R3+R4)
420 D=(R2+R4-R1-R3)^2+4*R3*R4
430 C=SQR(D)
440 W1=(B+C)/2
450 W2=(B-C)/2
460 B1=-(R1+R3)
470 B2=R3
480 B3=R4
490 B4=-(R2+R4)
500 C1=B2/(W1-B4)
510 C3=B3/(W1-B1)
```

```
520 C4=B3/(W2-B1)
530 A4=(A0-(B0*C3))/(C4-C3)
540 A3=B0-A4
550 A1=C3*A3
560 A2=A0-A1
570 FOR G=0 TO H
580 T5=G*M
590 IF W2*T5<-40 THEN 503
600 F1=A1*EXP(W1*T5)+A2*EXP(W2*T5)
610 F2=A3*EXP(W1*T5)+A4*EXP(W2*T5)
620 GO TO 510
630 IF W1*T5<-40 THEN 509
640 F1=A1*EXP(W1*T5)
650 F2=A3*EXP(W1*T5)
660 GO TO 510
670 S=0
680 S=F1+F2
690 IF S<1E-25 THEN 560
700 D3=(S*COS(2*3.142*(T5/F)))*M
710 D4=(S*SIN(2*3.142*(T5/F)))*M
720 A=A+D3
730 B=B+D4
740 NEXT G
750 A=A*2/F
760 B=B*2/F
770 L=2/(3.142)*(A*SIN(P)+B*COS(P))
780 PRINT#1:T,L
790 NEXT I
800 PRINT#1:"1E37","1E37"
810 PRINT "DONE"
820 END
```

EXSTBOX

```
100 REM    THIS PROGRAM SIMULATES THE OUTPUT OF A BOXCAR
110 REM  INTEGRATOR IN A DLTS RUN ON A GROUND-EXCITED STATE
120 REM  MODEL ELECTRON TRAP.  THE OUTPUT IS A DIGITIZED
130 REM  DATA CURVE READ INTO A FILE OF THE USERS CHOICE.
140 REM  A1C=GROUND STATE EMISSION RATE PREFACTOR
150 REM  A2C=EXCITED STATE PREFACTOR
160 REM  A12=COMMUNICATION PREFACTOR
170 REM  E1=GROUND STATE ENERGY
180 REM  E2=EXCITED STATE ENERGY
190 K=8.625E-5
200 PRINT "INPUT PREFACTORS A1C A2C,A12
210 INPUT F5,F6,F7
220 PRINT "RESULTS FILENAME?
230 INPUT A$
240 FILE#1:A$
250 PRINT "SCRATCH';    ';A$
260 INPUT B$
270 IF B$= NO" THEN 210
280 SCRATCH #1
290 PRINT A$;"    ;"SCRATCHED
300 PRINT "INPUT E1,E2
310 INPUT E1,E2
320 PRINT INPUT T1 T2 IN MILLISEC
330 INPUT T6,T7
340 T6=T6/1000
350 T7=T7/1000
360 T(1)=T6
370 T(2)=T7
380 PRINT "INPUT NORMALIZATION
390 INPUT N
400 PRINT "TEMPERATURE RANGE?
410 INPUT T1 T2
420 Q=(T2-T1)/100
430 FOR I=0 TO 100
440 A=E=D3=D4=0
450 T=T1+Q*I
460 A0=1/(1+EXP(-(E1-E2)/(K*T)))
470 B0=1-A0
480 R1=F5*T 2*EXP(-E1/(K*T))
490 R2=F6*T 2*EXP(-E2/(K*T))
500 R3=F7*EXP(-(E1-E2)/(K*T))
510 R4=f7
520 B=-(R1+R2+R3+R4)
530 D=(R2+R4-R1-R3) 2+4*R3*R4
540 C=SQR(D)
```

EXSTBOX (CONT'ED)

```
550 W1=(B+C)/2
560 W2=(B-C)/2
570 B1=-(R1+R3)
580 B2=R3
590 B3=R4
600 B4=-(R2+R4)
610 C1=B2/(W1-B4)
620 C3=B3/(W1-B1)
630 C4=B3/(W2-B1)
640 A4=(A0-(B0*C3))/(C4-C3)
650 A3=B0-A4
660 A1=C3*A3
670 A2=A0-A1
680 FOR G=1 TO 2
690 T5=T(G)
700 IF W2*T5<-40 THEN 650
710 F1=A1*EXP(W1*T5)+A2*EXP(W2*T5)
720 F2=A3*EXP(W1*T5)+A4*EXP(W2*T5)
730 GO TO 700
740 IF W1*T5<-40 THEN 690
750 F1=A1*EXP(W1*T5)
760 F2=A3*EXP(W1*T5)
770 GO TO 700
780 S=0
790 S=F1+F2
800 IF S<1E-25 THEN 730
810 S(G)=S
820 NEXT G
830 L=S(1)-S(2)
840 L=N*L
850 PRINT#1:T,L
860 NEXT I
870 PRINT#1:"1E37 , 1E37
880 PRINT "DONE"
890 END
```

OMEGA

```
100 REM    THIS PROGRAM PRINTS OUT THE INVERSE TIME CON-
110 REM  STANTS OF THE EXPONENTIAL TERMS IN THE SOLUTION OF
120 REM  THE COUPLED RATE EQUATIONS OF THE GROUND-EXCITED
130 REM  STATE ELECTRON TRAP MODEL.  THE COMMON RESULT BEING
140 REM  THAT ONE IS MUCH FASTER THAN THE OTHER.  THESE
150 REM  W S ARE THE INVERSE TIME CONSTANTS OF THE CAPACI-
160 REM  TIVE TRANSIENT AFTER THE INJECTION PULSE.
170 K=8.625E-5
180 PRINT  RESULTS FILENAME
190 INPUT A$
200 FILE#1:A$
210 PRINT "INPUT E1 E2
220 INPUT E1 E2
230 PRINT "INPUT STARTING TEMP
240 INPUT T2
250 PRINT  INPUT PREFACTORS
260 INPUT F5,F6,F7
270 PRINT#1: E1= ;E1, E2= ;E2
280 PRINT#1:"A1C= ;F5  A2C= ;F5  A12= ;F7
290 PRINT#1
300 PRINT#1
310 PRINT#1:"TEMP (K)", W+ ;"W-
320 FOR I=1 TO 10
330 T=T2+10*I
340 A1=F5*T 2*EXP(-E1/(K*T))
350 A2=F6*T 2*EXP(-E2/(K*T))
360 A3=F7*EXP(-(E1-E2)/(K*T))
370 A4=F7
380 B1=-(A1+A3)
390 B4=-(A2+A4)
400 W1=(B1+B4+((B1+B4) 2-4*(B1*B4-A3*A4)) .5)/2
410 W2=(B1+B4-((B1+B4) 2-4*(B1*B4-A3*A4)) .5)/2
420 PRINT T,W1;W2
430 PRINT#1:T,W1;W2
440 NEXT I
450 END
```

TRIXFIT

```
100 REM    THIS PROGRAM WILL PERFORM A LEAST SQUARES FIT
105 REM  ON A DATA FILE CONTAINING EXPERIMENTAL DATA IN
110 REM  THE FORM OF A DLTS PEAK.  THE FIT IS OF A SIMPLE
115 REM  SINGLE STATE TRAP WITH AN EXPONENTIAL EMISSION
120 REM  RATE.  THE CAPACITIVE TRANSIENT IS PROCESSED BY A
130 REM  SIMULATED LOCK-IN AMPLIFIER AND THEREFORE THE DATA
140 REM  MUST BE TAKEN FROM A DLTS SETUP USING A LOCK-IN
150 REM  AMPLIFIER.  THE PROGRAM IS INTERACTIVE WITH  DIGS
160 REM  AND MUST BE RUN ON A GRAPHICS TERMINAL.  AFTER A
170 REM  FIT IS DONE THE USER MAY CHOOSE TO REDEFINE THE
180 REM  STARTING PARAMETERS.  A MATRIX IS PRINTED SHOWING
190 REM  THE VALUES OF A FIT USING A RANGE OF PARAMETERS
200 REM  SPECIFIED BY THE USER.  THE PARAMETERS PRINTED BELOW
210 REM  THE MATRIX ARE THE BEST FIT PARAMETERS IN THE
220 REM  MATRIX.
230 DIM Q(800)
240 DIM X(200),Y(200),Z(200),W(200)
250 FOR J=1 TO 100
260 X(J)=Y(J)=Z(J)=W(J)=0
270 NEXT J
280 LIBRARY  L.IG***:TEKLEV0
290 LIBRARY  L.IG***:LEVEL1
300 LIBRARY  L IG***:TEKSUB3
310 PRINT 'NUMBER OF DIGITIZED DATA POINTS?
320 INPUT N1
330 PRINT "NAME OF DIGITIZED DATA FILE?
340 INPUT A$
350 FILE#1:A$
360 PRINT  DISPLAY THE FIT?
370 INPUT E$
380 DIM A(12,5)
390 FOR I=1 TO N1
400   INPUT#1:X(I),Y(I)
410 NEXT I
420 PRINT  SAVE RESULTS?
430 INPUT B$
440 IF B$= NO" THEN 480
450 PRINT "MATRIX RESULTS FILENAME?
460 INPUT C$
470 FILE#2:C$
480 PRINT  LOCK-IN FREQ F1,F2,P
490 INPUT J1 F1,F2,P
500 J1=1/J1
510 PRINT  ENERGY LIMITS?
520 INPUT E E3
```

TRIXFIT (CONT'ED)

```
530 PRINT "INITIAL PREFACTOR VALUE?
540 INPUT F
550 PRINT "PREFACTOR INCREMENT?
560 INPUT F3
570 IF E$= NO  THEN 630
580 FILE#3: *"
590 FOR I=1 TO N1
600 PRINT#3:X(I);Y(I)
610 NEXT I
620 PRINT#3:1E37;1E37
630 Q=3.14159
640 K=8.618E-5
650 S1=S3=-999
660 S2=999
670 C=2*Q*F2
680 R=COS(C)
690 U=SIN(C)
700 E1=(E3-E)/10
710 DEF FNS(Y)=(2/Q)*EXP(Y)
720 DEF FNB(X)=(((2*EXP(-B))/G)*(X*R-2*Q*U)-(2*X*M)/G+((M/Q)*U))*SIN(I
730 DEF FNA(X)=(((2*EXP(-B))/G)*(X*U+2*Q*R)-(4*Q*M)/G+(M/Q)*(1-R))*COS(P
740 DEF FNC(T)=F4*T^2*EXP(-E2/(K*T))
750 FOR I=2 TO 12
760 E2=E+(I-2)*E1
770 A(I,1)=E2
780 NEXT I
790 FOR N=2 TO 5
800 F4=F+(N-2)*F3
810 A(1,N)=F4
820 NEXT N
830 FOR I=2 TO 12
840 E2=E+(I-2)*E1
850 FOR N=2 TO 5
860      F4=F+(N-2)*F3
870      FOR J=1 TO N1
880        GO SUB 1430
890         IF S>S1 THEN 910
900        GO TO 920
910        S1=S
920      NEXT J
930      FOR J=1 TO N1
940        GO SUB 1430
950        Z(J)=Z(J)/S1
960      NEXT J
970      T1=0
980 FOR J=1 TO N1
990        X2=((Y(J)-Z(J)) 2)/(1+Z(J) 2)
1000        T1=T1+X2
1010      NEXT J
```

TRIXFIT (CONT'ED)

```
1020      A(I,N)=T1
1030 IF A(I,N)<S2 THEN 1050
1040 GO TO 1080
1050 S2=A(I,N)
1060 I1=I
1070 N2=N
1080   NEXT N
1090 NEXT I
1100 IF E$= YES  THEN 1120
1110 GO TO 1330
1120 E2=A(I1 1)
1130 F4=A(1,N2)
1140 PRINT E2;F4
1150 FOR J=1 TO 100
1160 T=70+(J*1)
1170 GO SUB 1440
1180 IF S>S3 THEN 1200
1190 GO TO 1210
1200 S3=S
1210 NEXT J
1220 FOR J=1 TO 99
1230 T=150+(J*1)
1240 GO SUB 1440
1250 W(J)=Z(J)/S3
1260 PRINT#3:T; ", ;W(J)
1270 NEXT J
1280 PRINT#3:1E37;1E37
1290 RESET #3
1300 CALL "TEKSUB3":#3
1310 SCRATCH #3
1320 CALL "ER":Q()
1330 MAT PRINT A
1340 PRINT
1350 PRINT E2;"  ";F4
1360 PRINT "ANOTHER E,A?
1370 INPUT F$
1380 IF F$= NO" THEN 1420
1390 PRINT "INPUT ENERGY VALUES, INITIAL A& INCREMENT
1400 INPUT E,E3,F,F3
1410 GO TO 570
1420 GO TO 1570
1430 T=X(J)
1440 D=FNC(T)
1450 X=D*J1
1460 IF X<80 THEN 1480
1470 X=80
1480 IF X>1E-10 THEN 1500
1490 X=1E-10
1500 A=F1*X
```

TRIXFIT (CONT'ED)

```
1510 B=F2*X
1520 M=EXP(-X)
1530 G=X^2+4*(Q 2)
1540 S=FNS(A)*(FNA(X)+FNB(X))
1550 Z(J)=S
1560 RETURN
1570 IF B$= NO" THEN 1630
1580 PRINT#2:A$
1590 PRINT#2:
1600 MAT PRINT#2:A
1610 PRINT#2:
1620 PRINT#2:
1630 END
```


DAT
FILM
2-8