COMPUTATIONAL SEPARATION OF BULK AND SURFACE RECOMBINATION USING CONTACTLESS PHOTOCONDUCTIVE DECAY

Frederick P. Giles
Purdue University School of Electrical and Computer Engineering

Richard J. Schwartz
Purdue University School of Electrical and Computer Engineering

Follow this and additional works at: http://docs.lib.purdue.edu/ecetr

http://docs.lib.purdue.edu/ecetr/102

This document has been made available through Purdue e-Pubs, a service of the Purdue University Libraries. Please contact epubs@purdue.edu for additional information.
COMPUTATIONAL SEPARATION OF BULK AND SURFACE RECOMBINATION USING CONTACTLESS PHOTOCONDUCTIVE DECAY

FREDERICK P. GILES
RICHARD J. SCHWARTZ

TR-ECE 96-6
APRIL 1996

SCHOOL OF ELECTRICAL AND COMPUTER ENGINEERING
PURDUE UNIVERSITY
WEST LAFAYETTE, INDIANA 47907-1285
COMPUTATIONAL SEPARATION OF

BULK AND SURFACE RECOMBINATION

USING CONTACTLESS PHOTOCONDUCTIVE DECAY

Frederick P. Giles
Richard J. Schwartz

School of Electrical Engineering
1285 Electrical Engineering Building
Purdue University
West Lafayette, IN 47907-1285

Research support provided by Sandia National Laboratories
# TABLE OF CONTENTS

| LIST OF TABLES | vi |
| LIST OF FIGURES | vi |
| ABSTRACT | x |

## CHAPTER 1: MEASUREMENT OF CARRIER RECOMBINATION

1.1 Introduction ........................................................................ 1
1.2 Introduction to Contactless Photoconductive Decay Techniques ........ 1
  1.2.1 Heuristic description of photoconductive decay .................... 2
  1.2.2 The microwave-detected PCD technique ............................... 3
  1.2.3 The inductively-coupled PCD technique ............................... 6
  1.2.4 The advantages of contactless PCD techniques ....................... 7
1.3 The Relevance of Lifetime Measurements to Solar Cells .................. 7
1.4 The Motivation for Separating Bulk and Surface Recombination ....... 8
1.5 A Brief Survey of Strategies Used to Distinguish Bulk and Surface Recombination ......................................................... 8
  1.5.1 Immersion of samples in special solutions to eliminate surface recombination .............................................................. 9
  1.5.2 Use of a pair of excitation sources to create different initial carrier profiles ................................................................. 9
  1.5.3 Passivation of surface states by ion deposition ....................... 9
  1.5.4 Separation of bulk and surface recombination by \textit{modulated} excitation source .............................................................. 10
1.6 Thesis Outline .................................................................... 10

## CHAPTER 2: PHOTOCONDUCTIVE DECAY MEASUREMENT THEORY

2.1 Introduction .......................................................................... 11
2.2 Effective Lifetime PCD Theory .................................................... 11
2.3 Microwave-detected PCD Theory ................................................. 13
<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.4 Inductively-coupled PCD Theory</td>
<td>17</td>
</tr>
<tr>
<td>2.5 General PCD Excess Carrier Distributions</td>
<td>19</td>
</tr>
<tr>
<td>2.6 Chapter Summary</td>
<td>22</td>
</tr>
<tr>
<td>Chapter 3: CONSIDERATION OF MICROWAVE-DETECTION PHENOMENA</td>
<td>23</td>
</tr>
<tr>
<td>3.1 Introduction</td>
<td>23</td>
</tr>
<tr>
<td>3.2 Excess Carrier Distribution Effects</td>
<td>24</td>
</tr>
<tr>
<td>3.2.1 Sensitivity to carrier distributions normal to surfaces</td>
<td>24</td>
</tr>
<tr>
<td>3.2.2 Lateral carrier diffusion</td>
<td>27</td>
</tr>
<tr>
<td>3.2.3 Reflectance dependence upon diffusion parallel to surfaces</td>
<td>28</td>
</tr>
<tr>
<td>3.2.4 Time-dependent microwave scattering</td>
<td>31</td>
</tr>
<tr>
<td>3.3 Summary of Results</td>
<td>34</td>
</tr>
<tr>
<td>Chapter 4: STUDY OF EQUATION COMPONENTS FOR THE PURPOSES OF RECOMBINATION PARAMETER SEPARATION</td>
<td>37</td>
</tr>
<tr>
<td>4.1 Introduction</td>
<td>37</td>
</tr>
<tr>
<td>4.2 Depth-Insensitive PCD Theory. Generalized for Two Independent Surface</td>
<td>37</td>
</tr>
<tr>
<td>Recombination Velocities</td>
<td>37</td>
</tr>
<tr>
<td>4.2.1 Exponential decay coefficients</td>
<td>38</td>
</tr>
<tr>
<td>4.2.2 Decay eigenvalues</td>
<td>38</td>
</tr>
<tr>
<td>4.2.3 Term amplitudes</td>
<td>41</td>
</tr>
<tr>
<td>4.3 Study of Combinations of Equation Parameters</td>
<td>41</td>
</tr>
<tr>
<td>4.3.1 Differences between adjacent eigenvalues</td>
<td>42</td>
</tr>
<tr>
<td>4.3.2 Differences of squared eigenvalues</td>
<td>43</td>
</tr>
<tr>
<td>4.3.3 Ratio of second and first amplitudes</td>
<td>45</td>
</tr>
<tr>
<td>4.3.4 The combination of $C_2/C_1$ with $k_2 - k_1$</td>
<td>47</td>
</tr>
<tr>
<td>4.4 Conclusion</td>
<td>49</td>
</tr>
<tr>
<td>Chapter 5: SEPARATION ALGORITHM</td>
<td>51</td>
</tr>
<tr>
<td>5.1 Introduction</td>
<td>51</td>
</tr>
<tr>
<td>5.2 Reasoning Behind the Algorithm</td>
<td>51</td>
</tr>
<tr>
<td>5.3 The Recombination Parameter Separation Process</td>
<td>52</td>
</tr>
<tr>
<td>5.3.1 Extraction of the decay parameters from the PCD curve</td>
<td>52</td>
</tr>
<tr>
<td>5.3.2 Deduction of the recombination parameters</td>
<td>52</td>
</tr>
<tr>
<td>5.4 The Separation Algorithm</td>
<td>53</td>
</tr>
<tr>
<td>5.4.1 The reasoning used to construct the algorithm</td>
<td>53</td>
</tr>
</tbody>
</table>
### LIST OF TABLES

<table>
<thead>
<tr>
<th>Table</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.1 Reflectances of equilibrium samples with added single plane conductive layers. Left column gives the conductivity, thickness, and location of the layer (see Fig. 1). Equilibrium conductivity of each sample is 0.02 S/cm; the overall sheet conductances of each sample are equal.............................,26</td>
<td></td>
</tr>
<tr>
<td>3.2 Reflectance of equilibrium samples with added planar conductive layers. Left column gives the conductivity, thickness, and location of the layer (see Fig. 1). Equilibrium conductivity of each sample is 0.2 S/cm; the overall sheet conductances of each sample are equal.............................,26</td>
<td></td>
</tr>
<tr>
<td>3.3 Area-weighted reflectance of a sample (background conductivity = 0.02 Siemens/cm) when conductive disks of various areas are embedded in it. (Top row shows the percentage of the total sample area occupied by the embedded disk; the left-most column gives the excess conductivity of the embedded disk when it is the same size as the sample.),30</td>
<td></td>
</tr>
<tr>
<td>3.4 Area-weighted reflectance of a sample (background conductivity = 0.2 Siemens/cm) when conductive disks of various areas are embedded in it. (Top row shows the percentage of the total sample area occupied by the embedded disk; the left-most column gives the excess conductivity of the embedded disk when it is the same size as the sample.),30</td>
<td></td>
</tr>
<tr>
<td>6.1 ESPRIT and separation results for the various curves in fig. 6.7; paired sets of results are in descending order, as in fig. 6.7. Curve fits calculated from decay parameters ((C_i, k_i)) are shown in figs. 6.9 through 6.13,..................,68</td>
<td></td>
</tr>
<tr>
<td>6.2 Measured effective lifetimes for conditions of fig. 6.7, measured at Sandia National Laboratories. Values were measured between 50 and 100 (\mu)s, rather than between 0 and 50 (\mu)s as in fig 6.7,.................................,68</td>
<td></td>
</tr>
</tbody>
</table>
**LIST OF FIGURES**

<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.1</td>
<td>Heuristic view of the equilibration of excess carriers by diffusion and recombination subsequent to a pulse of above-band-gap light from a laser diode</td>
<td>2</td>
</tr>
<tr>
<td>1.2</td>
<td>Example of excess carrier equilibration in the direction normal to the sample surfaces (across the smallest dimension of the sample). There are five time steps, distinguishable by their decreasing amplitudes on the left side of the plot. Parameter values are: bulk lifetime=1e-3 secs, left side SRV (surface recombination velocity)=20 cm/s, right side SRV=200 cm/s, diffusion constant =12 cm²/sec, sample thickness= 400 µm</td>
<td>3</td>
</tr>
<tr>
<td>1.3</td>
<td>Diagram of the Sandia Labs μW-PCD apparatus (from [1])</td>
<td>4</td>
</tr>
<tr>
<td>1.4</td>
<td>Diagram of the IC-PCD apparatus (from [45])</td>
<td>6</td>
</tr>
<tr>
<td>2.1</td>
<td>The solid line is a qualitatively correct simulated PCD decay curve (semilogarithmic). The dashed line shows the single-exponential decay which the PCD decay is asymptotically approaching</td>
<td>12</td>
</tr>
<tr>
<td>2.2</td>
<td>Side view of the basic geometry of the PCD microwave-detection section</td>
<td>15</td>
</tr>
<tr>
<td>2.3</td>
<td>Power reflectance vs. uniform conductivity in silicon for a four-medium system composed of air/Si (300 microns)/air (0.5 cm.)/Copper. The incident angle of the transverse electric plane waves is about 43 degrees, corresponding to waves of frequency 9.6 GHz propagating along a 1 by 2.2 cm TE₁₀ waveguide</td>
<td>16</td>
</tr>
<tr>
<td>2.4</td>
<td>Power reflectance vs. uniform conductivity in Silicon for a series of different reflector plate spacings. (All parameters are the same as in fig. 2.3.) The plate spacings vary from zero (the topmost curve) to 0.5 cm (lowest curve) in increments of 0.1 cm</td>
<td>17</td>
</tr>
</tbody>
</table>
2.5 Excess Camer Distributions within a measurement sample at 0, 10^{-6}, 10^{-5}, 10^{-4} and 10^{-3} seconds after cessation of the excitation; height of the leftmost side of the curve indicates temporal priority. Bulk lifetime is $10^{-3}$ secs.; there is no surface recombination. Diffusivity is 35 cm$^2$/s; absorption coefficient is $1000$/cm; sample width is 300 microns. This figure is jagged because it was computed using a finite number of terms from the infinite series representation of Eqn. 2.15..........................20

2.6 A time progression of carrier profiles for infinite SRVs at both surfaces, bulk lifetime of 1 millisecond. Profiles are for time = 0, 10^{-6}, 10^{-5} seconds. Thirty, five, and one Fourier term(s) are used, respectively, which accounts for the jaggedness. Diffusivity is $35$ cm$^2$/s; absorption coefficient is $1000$/cm; sample width is 300 microns.............................. 21

3.1 Excess conductive layer positions within a sample..........................25

3.2 Relative disk areas for the surface-parallel diffusion study, (area: are to scale.)...29

3.3 Polar scattering of 9.6 GHz microwaves normally incident on the face of a disk-shaped conducting region, 300 $\mu$m thick, with radius 0.4 cm. Surrounding medium is air........................................ 32

3.4 Plot of the first quotient term in the polar scattering function of eqn. 3.3............33

3.5 The second quotient term in the scattering function of eqn. 3.1...................34

4.1 Normalized eigenvalues (indices=1,2,3) vs. the base-10 logarithm of surface recombination velocity for W=400 microns, D=20 cm$^2$/sec..................40

4.2 Eigenvalue spacings vs. S (where $S_1=S_2=S$); W=400 microns, D=20 cm$^2$/sec.42

4.3 Squared eigenvalue differences $a_i^2 - a_{i+1}^2$, $j = i + 1$ (for i=0,1,2,3) vs. S; W=400 microns, D=20 cm$^2$/sec............................................... 43

4.4 A plot of the normalized difference between second and first decay coefficients $W^2 (k_2 - k_1)/D_p = (\alpha_2^2 - \alpha_1^2)W^2$ versus $\{S_1,S_2\}$ for W = 400 $\mu$m
and $D_p = 12.8$ cm$^2$/sec........................................... 44

4.5 The amplitude ratio surface $C_2/C_1$ vs. the SRVs, using the values
W = 400 $\mu$m, $D_p = 12.8$ cm$^2$/sec, and $y = 294$/cm.............................45

4.6 The amplitude ratio surface $C_2/C_1$ vs. the SRVs, using the values
W = 400 $\mu$m, $D_p = 12.8$ cm$^2$/sec, and $y = 11.8$/cm.............................46
4.7 The amplitude ratio surface \( C_2/C_1 \) vs. the SRVs, using the values 
\[ W = 400 \mu \text{m}, \quad D_p = 12.8 \text{cm}^2/\text{sec}, \quad \text{and} \quad \gamma = 7000/\text{cm}. \]
\[ \text{........................................}47 \]

4.8 Some representative level curves of \( k_2 - k_1 \) from fig. \[ \text{........................................}48 \]

4.9 Some representative level curves of \( C_2/C_1 \) from fig. \[ \text{........................................}49 \]

5.1 Flow diagram for the separation algorithm,\[ \text{........................................}56 \]

6.1 The appearance of a measured microwave-detected PCD decay curve,\[ \text{........................................}60 \]

6.2 Measured \( \mu \text{W-PCD} \) data; sample and sampling parameters as displayed,\[ \text{........................................}61 \]

6.3 \text{Semilog} plot of the \( \mu \text{W-PCD} \) data from fig. 6.2,\[ \text{........................................}62 \]

6.4 A measured \( \mu \text{W-PCD} \) decay with small surface recombination velocities,\[ \text{........................................}63 \]

6.5 \( \mu \text{W-PCD} \) curve with 0.2 Suns red-light bias,\[ \text{........................................}64 \]

6.6 An inductively-detected PCD measurement curve; noise on the right of the figure is due to digitization error,\[ \text{........................................}65 \]

6.7 Five pairs of front/back side \( \mu \text{W-PCD} \) measurement pairs. The laser drive currents, in descending order, are \[ 40 \text{ mA}, \quad 35 \text{ mA}, \quad 30 \text{ mA}, \quad 25 \text{ mA}, \quad 20 \text{ mA}. \]
The upper curve of each pair had the incident beam on the polished side of the sample,\[ \text{........................................}67 \]

6.8 (a) The upper diagram depicts the equilibrium condition of a lightly doped p-type sample with positive fixed oxide charge. (b) The lower figure depicts the condition of the same material, just after excitation has flattened the surface bands. (Free carriers in bands not shown.)\[ \text{........................................}70 \]

6.9 The curves of highest amplitude (40 mA laser drive current) from fig. 6.7, and their fit curves. The fitted curves extend past the end of the measured curves for identification purposes,\[ \text{........................................}71 \]

6.10 The curves of second highest amplitude (35 mA laser drive current) from fig. 6.7, and their fit curves. The fitted curves extend past the end of the measured curves for identification purposes,\[ \text{........................................}72 \]

6.11 The curves of third highest amplitude (30 mA laser drive current) from fig. 6.7, and their fit curves. The fitted curves extend past the end of the measured curves for identification purposes,\[ \text{........................................}73 \]

6.12 The curves of fourth highest amplitude (25 mA laser drive current) from fig. 6.7, and their fit curves. The fitted curves extend past the end of the measured curves for identification purposes,\[ \text{........................................}74 \]
6.13 The curves of lowest amplitude (20 mA laser drive current) from fig. 6.7, and their fit curves. The fitted curves extend past the end of the measured curves for identification purposes.

A novel, computational approach to distinguishing between bulk and surface recombination in crystalline silicon is presented. The Photoconductive Decay technique, applied with a probe of sufficiently long wavelength, senses no information about carrier diffusion or distributions in samples, thus isolating carrier recombination as the sole cause of its decay signal. If the recombination and transport parameters of a sample remain constant during the decay, the information content and collective properties of the decay parameters allow them to be solved simultaneously to produce unique values for the bulk lifetime and surface recombination velocities of the measurement sample. The method is rapid and simple, requires no special sample preparations or equipment, and does not alter samples. The method is demonstrated on measured data.
1. MEASUREMENT OF CARRIER RECOMBINATION

1.1. Introduction

In this work, a method is sought by which bulk and surface recombination can be separated by computations on measurement data from contactless photovoltaic (PCD) decay techniques. If a computational method of separating recombination components can be found, it would inherit the beneficial properties possessed by the contactless PCD techniques of not destroying or modifying measurement samples, not requiring electrical contacts on the sample (which enables measurements at any phase of production), as well as requiring few additional equipment costs, making it a simple enhancement to any existing commercial or prototype apparatus. It is hoped that such a method would be rapid, simple, and accurate as well. The following sections introduce the subject of lifetime measurements on solar cells, contactless photoconductive decay techniques, and methods of separating recombination components.

1.2 Introduction to Contactless Photoconductive Decay Techniques

Photoconductive decay (PCD) is a family of related lifetime measurement techniques that utilizes a transient decay of light-generated excess carriers to produce an associated detection response from which the desired recombination parameter(s) can be extracted. Since photoconductivity in a semiconductor is a property dependent upon mobile free carriers, the time-dependence of the photoconductivity is directly related to the recombination rates of the carriers. There exist both electrically-detected and contactless varieties of the PCD technique.

There are two major variations of contactless PCD which have found comparable amounts of use, as indicated by their publication histories. One method detects the decay of the photoexcited excess carriers by the microwave reflectance produced. The other method places a radio-frequency inductive loop (connected to a bridge circuit) near the measurement sample, and senses the photoconductivity by the imbalance of the bridge. (Capacitive coupling is a third method of contactless PCD detection [4], but has not found much use, and therefore will not be considered here.)
1.2.1 Heuristic description of photoconductive decay

PCD is conceptually very simple. A description of the "photoconductive decay" aspect common to the contactless techniques is as follows. Applying a pulse of above-band-gap light to a semiconductor sample creates excess electron-hole pairs that increase its conductivity for the duration of their existence, as visualized in the time sequence in figures 1.1 and 1.2 below. Carriers generated in a limited locale diffuse in all directions within the sample, recombining at the surfaces and within the material. The initial carrier gradients normal to the sample surfaces (figure 1.2) depend upon the wavelength (and the absorption coefficient) of the generating laser, with higher energy photons creating a steeper initial gradient. Initial carrier gradients parallel to the sample surface depend upon the transverse intensity profile of the beam (i.e., the laser "spot size"). (Chapter 2 describes the carrier distributions quantitatively.)

![Fig. 1.1: Heuristic view of the equilibration of excess carriers by diffusion and recombination subsequent to a pulse of above-band-gap light from a laser diode.](image-url)
1.2.2 The microwave-detected PCD technique

The microwave-detected version of PCD (μW-PCD) takes place as follows. When the conductivity of the measurement sample is temporarily increased, its microwave absorbing and reflecting properties change accordingly (since the dielectric constant's (phasor) imaginary component is proportional to the conductivity). In other words, when the sample is in equilibrium it will reflect a constant percentage of the impinging microwave energy, but when the sample contains an excess of decaying carriers, the reflected microwaves will vary with a time-dependence that is related to the excess conductivity present. Since carrier (and conductivity) decay in the sample is determined by the recombination and transport parameters of the sample, the microwave reflectance decay data contains this decay information, though perhaps in a more complicated form. Therefore, by continuously directing microwaves towards a post-excited sample and recording the time-dependence of the reflected microwave energy, a time decay curve is
Fig. 1.3: Diagram of the Sandia Labs μW-PCD apparatus (from [1]).
obtained that ostensibly allows the measurement of the recombination and transport parameters of the sample.

Figure 1.3 is the diagram of a typical $\mu$W-PCD apparatus (the one employed at Sandia National Laboratories [1]). The physical configuration places a measurement sample over the opening of a vertically oriented hollow, rectangular $\text{TE}_{10}$ mode waveguide. The measurement sample is kept within a light-insulated enclosure so that it receives no ambient light. Single mode (usually $\text{TE}_{10}$ mode) microwaves are continuously guided toward the measurement sample. (The $\text{TE}_{10}$ mode has electric field strictly transverse to the direction of wave propagation in the waveguide, with one half-period of sinusoidal electric field variation across the widest transverse dimension of the guide.)

Consider now a trial of the $\mu$W-PCD technique. The pulse of a GaAs diode laser generates electron/hole pairs in a spot on the sample at the center of the waveguide opening. Probing microwaves are continuously guided towards and reflected from the excited region and its surrounding vicinity. The excess carriers embody a brief, localized conductivity transient within the sample, which in turn stimulates a microwave reflectance transient. A square-law detector within the waveguide senses this microwave transient, with the decaying voltage output from the detector sampled and stored in a digital oscilloscope. To increase the signal-to-noise ratio of the reflectance curve, a large number of these trials are performed and averaged. An effective carrier lifetime is then inferred from this averaged reflectance curve through a computer curve fit.

$\mu$W-PCD [1,2,3] is presently in use at many research laboratories throughout the world, and several commercial apparatuses are available. (In the literature, a virtually identical technique is known by the name of Time-Resolved Microwave Conductivity (TRMC) [5, 6].) One group, the Photovoltaic Device Fabrication Laboratory at Sandia National Laboratories, has utilized a commercial $\mu$W-PCD apparatus for the past few years to measure carrier lifetimes for production-line solar cell quality control [1]. The apparatus was modified to perform measurements and extract results under computer control, and has been shown to be rapid and reliable for the vast majority of measurement samples.

This version of PCD has been applied to many materials, including HgCdTe [7], GaAs [8-12], AlGaAs [13], InP [8,14], CIS materials [15], polycrystalline silicon [16], amorphous silicon [17-19], and crystalline silicon [1, 5, 6]. Although most often used to make carrier lifetime measurements, it has also been used to measure carrier mobilities, as well as to make spatial maps of carrier lifetimes in samples.
1.2.3 The inductively-coupled PCD technique

The inductively-detected version of PCD (IC-PCD) is effectuated in the following manner [44]. The coil portion of an RLC circuit is placed near the measurement sample, with the plane of the coil’s opening placed parallel to the sample’s broad surface. A radio-frequency voltage is imposed upon the coil, creating time-varying magnetic fields which in turn produce eddy currents in the sample. The resistivity of the sample is thus detected as an added resistance in the coil by reason of the proximity of the sample to the coil.

The circuitry in which the coil is placed may consist of either an RLC tank circuit or a radio-frequency (RF) bridge. In the RLC tank circuit, the effect of the photoconductive decay in the sample is to induce a time-varying Q of the tank circuit. Under proper calibration conditions, the amplitude of the tank circuit voltage is proportional to this variation of Q, producing a voltage that can be recorded on an oscilloscope. In the RF bridge circuit implementation, the photoconductive decay takes the bridge out of balance, producing an error voltage which can be recorded.

![Diagram of the IC-PCD apparatus](from [45]).

Figure 1.4 shows the form of the apparatus used at the National Renewable Energy Laboratory (NREL.) For a particular sample, the coil-to-sample distance is fixed and then the bridge is balanced to null out the effect of the dark conductivity of the sample. The excitation pulse applied to the sample increases the sheet conductance of the sample,
causing the resistance of the sample to decrease, imbalancing the bridge. This RF error signal is mixed down to DC, amplified, and then sampled by a digital processing oscilloscope. Multiple trials and averaging are used to decrease the noise present in the final data. IC-PCD has found widespread use [25, 26, 46-50].

1.2.4 The advantages of contactless PCD techniques

The contactless PCD techniques described above have distinct advantages over lifetime measurement techniques which require electrical contacts on their measurement samples. The fabrication sequence of most crystalline silicon devices, including solar cells, begins with a boule of doped, crystalline silicon that is sliced into wafers to provide the basic material for devices. The devices are then created in (and on) these wafers by subjecting batches of them to a sequence of thermal oxidations, selective acid etching steps, high-temperature dopant diffusions, and other processes. One of the final steps in the device fabrication sequence is generally the deposition of electrical contacts on the devices, which must be present for electrically-detected measurements to be taken. For this reason, measurements requiring electrical contacts can usually only be taken from completed devices unless extra, intermediate steps are added to the normal fabrication sequence. In contrast, contactless PCD techniques can be applied without regard to whether contacts have been added to a device or sample, making them capable of measuring lifetime on devices at any stage of processing, on boules of starting material, and on bare wafers. Thus, they can be used to screen for and select high quality starting wafers, assess the effects of processing conditions upon device quality, and monitor the cleanliness of furnace tubes for manufacturing quality control purposes. These features make contactless PCD a very useful all-around tool for producing high-performance solar cells.

1.3 The Relevance of Lifetime Measurements to Solar Cells

The ability to measure the recombination rates of materials is important for solar cells, whose performance depends upon their ability to collect the maximum number of photogenerated charge carriers. Low recombination rates translate into the ability of free carriers to travel long distances within cells, which is required for the maximum number of these carriers to be collected. In crystalline silicon solar cells, the low-level injection recombination rates are set by the Shockley-Read-Hall (SRH) mechanism (also known as phonon-assisted recombination). SRH recombination rates increase with the concentration of impurities (usually metal ions) and imperfections (vacancies, dislocations, interstitials) in the cell; these flaws tend to accumulate during the high-temperature processing steps and by the inadvertent incorporation of contaminants that may have built up in the processing
environment over time. To produce solar cells with top performance, the best course of action is to select starting wafers of the highest quality, and to continually maintain a non-
contaminating processing environment, while employing a processing sequence which minimizes the damage inflicted upon the material. Contactless photoconductive decay techniques are useful tools for performing tests that can ensure these materials and processing criteria.

1.4 The Motivation for Separating Bulk and Surface Recombination

The main figure of merit for solar cells is their power conversion efficiency, the power produced by the cell over the amount of optical power presented to the cell. The parameter which limits the conversion efficiency of modern crystalline silicon solar cells is the open-circuit voltage, which depends mainly upon carrier recombination in the device. To increase the open-circuit voltage, it is required that recombination rates in completed devices be as low as possible; however, it is not always clear whether recombination in the interior (bulk) region of the device or recombination at the surfaces of the device is to blame for limiting performance.

Most lifetime measurement procedures produce only a single figure, the "effective lifetime" of measurement samples, which is a conglomeration of bulk and surface recombination and device effects and will often differ for different techniques. While the effective lifetime gives useful information about recombination, it is even more desirable to be able to separate the effects of recombination in the bulk region of a sample from that which is occurring at its surfaces. A sample with a long bulk lifetime and very poor quality surfaces might have the same effective lifetime as a different sample with a poor bulk lifetime and well-passivated surfaces. The methods used to treat the bulk and surface regions of the material are very different, so that knowledge about where the recombination is occurring is required to deal with it effectively. For this reason, a recent objective of carrier lifetime measurement techniques has been a search for methods by which to distinguish between bulk and surface recombination.

1.5 A Brief Survey of Strategies Used to Distinguish Bulk and Surface Recombination

A number of methods have been proposed for distinguishing between the surface recombination and the bulk (volume) recombination of semiconductors. However, all of them require multiple measurements, and most of them require complicated surface preparations, expensive additional equipment, or sacrificial measurement samples. For
purposes of comparison with the proposed computational method, the predominant separation methods are briefly described below.

1.5.1 Immersion of samples in special solutions to eliminate surface recombination

Yablonovitch and coworkers [26] have demonstrated that the immersion of samples in a bath of hydrofluoric acid effectively passivates all surface states, reducing their surface recombination velocities to below 1 cm/sec. With this strategy, one would take a normal, effective lifetime measurement whose result contains both bulk and surface recombination, and then an immersed measurement whose result includes only bulk recombination. The second measurement would give the true bulk lifetime, and the surface recombination could then be arrived at by subtraction.

This simple scheme is widely used with the inductively-coupled PCD technique; however since it removes the oxide from samples, it is obviously destructive to normal fabrication processes, and for production-line monitor usage, would only be applicable to test wafers. In addition, it requires multiple measurements. More recently, M'Saad and coworkers [55] have suggested the use of an Iodine/Methanol solution to accomplish the passivation of surface states.

1.5.2 Use of a pair of excitation sources to create different initial carrier profiles

Kunst and coworkers [36] demonstrated how surface and bulk recombination could be distinguished by sequential measurements using differently absorbed excitation lasers. The shorter wavelength source is absorbed more drastically in samples, which creates a higher proportion of carriers near the excited surface, thus causing a distribution that is initially more sensitive to surface recombination at that surface. Thus, taking measurements with each of the sources allows one to deduce the contributions to surface and bulk recombination by comparison. This technique is non-destructive, requires multiple measurements and adds the additional cost of a second excitation laser.

1.5.3 Passivation of surface states by ion deposition

More recently, Schofthaler and coworkers have described a method for passivating surface states by depositing ionized molecules on the exterior oxide of samples [42]. This technique is non-destructive, yet requires multiple measurements and requires the equipment needed for producing the ionized molecules.
1.5.4 Separation of bulk and surface recombination by modulated excitation source

In previous work [51,52,53,54], Sanii and coworkers demonstrated how a modulated excitation source could be used to distinguish bulk and surface recombination. In optically excited starting wafers, carrier transport is by diffusion (that is, it is caused by concentration gradients). When the intensity of the optical excitation is modulated rather than constant, bulk diffusion gradually disappears as the period of the excitation modulation decreases to near (and below) the effective lifetime of the wafer. (This cessation of carrier diffusion is responsible for the cutoff frequencies of diodes and other junction devices and is referred to as diffusion capacitance.) The effect upon a lifetime measurement of this kind of excitation is that carrier distributions can be made selectively shallower from the excited surface, which allows for different emphases upon the surfaces and bulk recombination.

The typical measurement procedure is to split the probe beam prior to its entrance into the sample to provide a reference signal. Feeding these probe and reference signals into the differencing inputs of a lock-in amplifier creates both amplitude and phase signals. The amplitude curve rolls off at a characteristic corner frequency, while the phase signal gradually shifts. By self-consistent fitting techniques, these curves characterize the bulk and surface recombinations in a sample.

1.6 Thesis Outline

To begin, Chapter 2 will present the general theory of contactless PCD with two independent surface recombination velocities in junctionless samples, assuming that the carrier distributions only along one spatial dimension are important. Chapter 3 will examine some of the widely held (but heretofore unjustified) assumptions about the PCD theory, including one-dimensionality of carrier distributions and other factors that could contribute to the shape of the general \( \mu \text{W-PCD} \) decay curve. In general, each of the phenomena considered are (undesirably) non-linear or non-constant.

Under the assumption that contactless PCD is able to isolate recombination as the sole cause of the PCD decay if the proper probe parameters have been selected, Chapter 4 will then specialize the PCD theory in order to discover an analytical foundation for the computational separation. Chapter 5 will then present the separation algorithm. Chapter 6 will apply the technique to measurement data, analyzing the results for validity. Chapter 7 will then summarize the findings of this research and suggest modifications and other studies by which this work might be furthered.
2. PHOTOCONDUCTIVE DECAY MEASUREMENT THEORY

2.1. Introduction

The theories pertaining to contactless photoconductive decay (PCD) techniques will be presented in this chapter. The simple and widely used "effective lifetime" picture of PCD will be described first, to give the reader an intuitive conception of PCD. This viewpoint ignores all but the asymptotic decay of the excess carriers in the sample, and thus does not consider the details of carrier diffusion and distributions in the excited sample.

The theory pertaining to microwave-detection of PCD is presented next, followed by the theory pertaining to inductively-coupled detection of PCD. Finally, the carrier distributions common to all monochromatic photoexcited samples are considered. In one-dimension, this is a Sturm-Liouville boundary-value problem which is solved by an infinite Fourier Series. The series contains all of the information about the carrier diffusion and recombination in post-excited PCD samples that was ignored in the first-order "effective lifetime" model.

2.2. Effective Lifetime PCD Theory

It is best to now consider the simple, first-order PCD theory, one that most authors use to extract an "effective lifetime" for the measurement sample. This streamlined theory disregards the initial portions of the PCD curve, considering it to be of dubious origin, and utilizes only the final, asymptotic portion (see figure 2.1, next page) to obtain recombination rate information.

To explain the theory of the technique, consider the excess carriers distributed across the thin dimension of the sample (along the axis normal to the sample surfaces). Just after a very brief excitation pulse (on the order of a nanosecond), the carrier distribution is approximately the exponential generation profile according to Beer's law. Thereafter, diffusion of the excess carriers towards the unexcited surface, along with simultaneous recombination, will cause them to rapidly settle into approximate homogeneity across the sample [9]. ("Approximate homogeneity" is the last stage of carrier decay in a thin sample in which diffusion has ceased (except that occurring to supply recombination...
processes at the surfaces), leaving recombination as the sole means of equilibration in the sample. In such cases, excess carrier concentrations are constant across samples in which there is no surface recombination, and possess gradients near the surfaces in cases where surface recombination is occurring.

The final portion of a PCD curve is due to excess carriers in approximate homogeneity, which approximately decays as a pure exponential function of time. The time constant of the decay is the "effective lifetime" of the sample. Figure 2.1 depicts the qualities of a typical PCD transient. The initial portion of the curve decays more rapidly than an exponential and asymptotically approaches a single exponential.

![Figure 2.1](image)

Fig. 2.1: The solid line is a qualitatively correct simulated PCD decay curve (semi-logarithmic). The dashed line shows the single-exponential decay which the PCD decay is asymptotically approaching.

Although the theory of PCD is greatly simplified when the initial, diffusive portion of the carrier equilibration is neglected, this also discards the information contained therein. Under the conditions of approximate homogeneity, the excess carrier decay is determined solely by bulk and surface recombination, and is described by [4]

$$\Delta p(t) = \Delta p_0 \exp(-t/\tau_{\text{eff}})$$  \hspace{1cm} (2.1)

where
\[ \frac{1}{\tau_{\text{eff}}} = \frac{1}{\tau_b} + D_p \alpha^2 \] (2.2)

\[ \tan(\alpha W) = \frac{2\alpha SD_p}{(\alpha^2 D_p^2 - S^2)} \] (2.3)

\( W \) is the sample thickness, \( S \) is the surface recombination velocity (assumed equal at the two surfaces), \( D_p \) is the minority carrier diffusion coefficient, and \( \tau_{\text{eff}} \) and \( \tau_b \) are the \textbf{effective} lifetime and bulk lifetime of the sample. The effective lifetime in eqns. 2.1 and 2.2 is generally a function of both the bulk and surface recombination of the sample. It can be seen that if \( S = 0 \), the effective lifetime is just the bulk lifetime of the sample, and if \( S \) becomes very large, the second term in eqn. 2.2 approaches the constant value \( D_p \left( \frac{\pi^2}{W^2} \right) \). With this basic understanding of the PCD, the theories of the detection methods can now be described.

\section*{2.3 Microwave-detected PCD Theory}

The theory of the microwave-detection of PCD is composed of a reflectance function that depends upon the geometry of the microwave system, the excitation conditions, and the material parameters of the sample. Because it employs higher frequencies than the inductively-coupled PCD method, the microwave version's electromagnetic skin depth is much shallower. An outline of the theory of this technique was presented in 1986 by Kunst and Beck [5]. In that work, the technique is referred to as the Time Resolved Microwave Conductivity (TRMC) technique, and \textit{differs} from the \( \mu \)W-PCD technique in that it generally employs higher frequency microwaves and may place the sample inside the waveguide. The theory presented in that work sketched the outline for consideration of carrier distributions in three-dimensions and inhomogeneous microwave fields, but presented only the details for simpler cases. In practice, most authors (see [21], for instance) extract the effective lifetime, as described above.

If the probing microwaves emanating from the open waveguide mouth behave approximately as one-dimensional plane waves, the percentage of microwave power reflected from a \( \mu \)W-PCD sample can be derived from wave-impedance theory [22]. The concept of wave impedance considers the description of uniform electromagnetic (EM) plane waves propagating through space as being analogous to electrical transmission lines that are sinusoidally excited. The electric fields of the microwaves are analogous to
voltages, while the magnetic fields are analogous to electrical currents. The transverse ratio of electric field to magnetic field is then a wave impedance, in units of ohms.

The wave impedance of a sample depends upon (among other things) its conductivity, which is now divided into two components: the conductivity due to the thermal equilibrium carrier concentrations (and which are fixed by doping and temperature), and the photo-excitiated conductivity due to excess carriers (and which depends upon the bulk lifetime, surface recombination velocities, and diffusivities of the sample.) It is this latter component of conductivity, through the chain of dependencies and the assumptions that prescribe their relationships, that the effective lifetime of a test sample is deduced from reflectance transient data.

To relate the excess carrier decay to the reflectance decay, the following chain of dependences is established. The total conductivity of the excited sample, separated into equilibrium and excess portions, is

$$\sigma = \sigma_0 + \Delta \sigma$$  \hspace{1cm} (2.4)

where

$$\Delta \sigma = q(\mu_n \Delta n + \mu_p \Delta p)$$  \hspace{1cm} (2.5)

$q$ is the unit of electron charge, the respective $\mu$ values are the conductivity mobilities of the excess electrons $n_e$, and the excess holes, $p_h$. In the absence of trapping, excess electrons and holes have nearly equal concentrations, so that eqn. 2.5 can be simplified as

$$\Delta \sigma = q(\mu_n + \mu_p) \Delta \rho.$$  \hspace{1cm} (2.6)

Next, consider the effect of this excess conductivity upon microwaves that impinge upon the measurement sample. The complex-valued permittivity of the sample [22] is in general

$$\varepsilon = \varepsilon_0 \varepsilon_{\text{rel}} - j \varepsilon_0 \frac{\sigma}{\omega}$$  \hspace{1cm} (2.7)

where $\omega$ is the radian frequency of the incident microwaves. Inserting the excess conductivity expression (2.6), into (2.4) and then placing this result in (2.7), the complex-valued permittivity is, more specifically,
By next resorting to wave-impedance theory, the overall reflectance of the system of media shown in figure 2.2 can be computed in stages by using the formulas for the wave-impedance of each medium. The general expression wave-impedance of each medium, for plane waves whose electric field is strictly transverse to their direction of propagation, is

$$
e = \varepsilon_0 \varepsilon_{rel} - j \frac{\sigma_0 + q(\mu_n + \mu_p) \Delta \rho}{\omega}$$  \hspace{1cm} (2.8)$$

where $\theta$ is the angle of incidence of the wave from the axis normal to the surface of the medium. The wave-impedance of the sample is then

$$Z_{\text{sample}} = \frac{\mu_0}{\varepsilon_0 \varepsilon_{rel}} \frac{\mu_0}{\eta \sec(\theta)}$$  \hspace{1cm} (2.9)$$

The net wave impedance of the system of figure 2.2 can then be determined by transforming the wave impedance of the metal plate (back towards the open mouth of the
waveguide) through the intervening air-gap, and repeating this process for the sample and the second air gap, using the "Smith chart" impedance transformation expression [22]

\[
Z_{\text{input}} = Z_{\text{adjacent}} \frac{Z_{\text{right}} \cos(kl) + jZ_{\text{adjacent}} \sin(kl)}{Z_{\text{adjacent}} \cos(kl) + jZ_{\text{right}} \sin(kl)}.
\]  

(\(Z_{\text{right}}\) refers to the net impedance of the system to the right of the boundary that is being transformed from, and \(Z_{\text{adjacent}}\) is the medium that is being transformed across.)

A representative example of the total reflectance of the system of figure 2.2, computed using the above procedure, is plotted in figure 2.3 as a function of the total, uniform conductivity of a silicon sample. The parameters used in the calculations were: sample thickness of 300 microns, two lossless air layers with unity dielectric constants, and an incident microwave frequency of 9.6 GHz. The spacing between the metal plate and the sample was chosen to obtain a curve of maximum sensitivity to changes in conductance (i.e., changes in reflectance having slopes of greatest magnitude everywhere).

![Power reflectance vs. uniform conductivity in silicon for a four-medium system composed of air/Si (300 microns)/air (0.5 cm)/Copper.](image)

As figure 2.3 shows, changes in the reflectance of measurement samples are non-linear functions of changes in conductivity. However, they are approximately linear for
small deviations from equilibrium conductivities [5]. Since the time-decay of excess carriers (and conductivity) in the "approximate homogeneity" regime follows an exponential decay law, if the reflectance function can be approximated as linear, the reflectance transient will also be a decaying exponential whose time constant is related to the effective lifetime of the sample. Also, the linearity of reflectance for a sample can be increased, if needed, at the sake of sensitivity (slope), as demonstrated in figure 2.4.

![Graph](image)

Fig. 2.4: Power reflectance vs. uniform conductivity in Silicon for a series of different reflector plate spacings. (All parameters are the same as in figure 2.3.) The plate spacings vary from zero (the topmost curve) to 0.5 cm (lowest curve) in increments of 0.1 cm.

### 2.4 Inductively-coupled PCD Theory

The inductive coupling method of PCD detection employs a small coil (usually about two turns) placed plane-parallel with the sample surface. When the coil is excited by an ac voltage, the time-varying magnetic field about the coil produces curling electric potentials (a la Faraday's law) near the coil. These potentials create eddy currents in the sample which appear as an (additional) ohmic loss across the terminals of the coil. This ohmic loss depends on the coil-to-sample distance and the ac oscillator frequency.

To increase the sensitivity of the coil's detecting abilities, it is placed in the reactive arm of a bridge circuit (which is excited by a radio-frequency (RF) oscillator.) The bridge is balanced for a sample's dark conductivity before a measurement is made, so that the photoconductivity is detected as it takes the bridge out of balance. Across the bridge is a
differential amplifier, whose output (the RF modulated PCD signal) is homodyned down to DC and sampled by a digital storage oscilloscope.

The skin depth of the inductively-coupled method is much greater than for the microwave-detected version because of the much lower electromagnetic frequencies employed [45]. This gives it an advantage for the present purposes in that it is far less sensitive to the conductivity distributions in the sample.

Assuming that there is no depth sensitivity at the RF frequency used, the power absorbed by the sample [44] is

$$ P = \left( \frac{k}{L} \right) V_L^2 G. \quad (2.12) $$

where \( k \) is a geometry and coupling constant, \( L \) is the inductance of the coil, \( V \) is the voltage across the coil, \( W \) is the sample thickness, and \( G \) is the conductance of the sample. Therefore, the PCD (excess) power dissipation is

$$ \Delta P = \left( \frac{k}{L} \right) V_L^2 \int_{0}^{W} (\Delta \sigma) dz \quad (2.13) $$

or (assuming that there are no traps in the material)

$$ \Delta P = \left( \frac{k}{L} \right) V_L^2 q \left( \mu_e + \mu_h \right) \int_{0}^{W} (\Delta \rho) dz. \quad (2.14) $$

where \( q \) is the unit electron charge, the \( \mu \) are the respective electron and hole mobilities, and \( \Delta \rho \) are the minority carriers (holes) in the material.

A trial of the technique is as follows. The sample is placed upon the measurement stage, and the coil-to-sample spacing is adjusted for high sensitivity. The reactive bridge arm is then balanced by adjusting the series capacitor, the RF oscillator frequency, and the coil-to-sample coupling distance. The sensitivity of the detection circuit to changes in the \( G \) of the sample is proportional to the \( Q \) of the resonant arm of the bridge [45]; thus, the coil-to-sample distance is varied depending upon the sample to obtain the highest sensitivity. The sample is excited by a low-power laser pulse which generates free carriers and takes the bridge out of balance. This produces an error signal which gradually disappears as the carriers diffuse and recombine. The error signal is continuously mixed down to baseband frequencies and sampled by the storage scope. Trials are repeated and averaged to decrease
the noise levels in the sampled signal. The effective lifetime is extracted as it was for the microwave method.

2.5 General PCD Excess Carrier Distributions

In section 2.1, the PCD "effective lifetime" theory of was presented; that theory utilized only the final, asymptotic portion of the PCD decay curve (due to carriers in "approximate homogeneity"), leaving the initial, steeper portion unexplained. This section will present the fundamental physical cause for the initial portion of PCD decay curve for depth-insensitive probes. (If the probe is sensitive to carrier distributions (e.g., 25 GHz microwaves), part of the initial PCD decay should also be attributed to time-dependence of the electromagnetic reflections from the equilibrating, non-simple carrier distributions in the sample or other non one-dimensional effects. Chapter 3 considers the other possible factors that might contribute to the early portion of the PCD decay for the microwave-detected version of the technique.)

In low-level carrier injection, the minority carrier diffusion equation (MCDE) is sufficient to describe the carrier distributions within the measurement sample. Considering only variations in carrier concentrations across the thicknesses of samples, and assuming constant recombination and transport parameters, the general solution of the MCDE is

$$\Delta p(x,t) = e^{-\gamma t} \sum_{i=1}^{\infty} e^{-D_p \alpha_i t} [A_i \cos(\alpha_i x) + B_i \sin(\alpha_i x)]$$

(2.15)

where the eigenvalues $\alpha_i$ may be found by solving the transcendental equation

$$\tan(\alpha_i W) = \frac{\alpha_i}{D_p} \left( \frac{S_1 + S_2}{\alpha_i^2 - \frac{S_1 S_2}{D_p^2}} \right)$$

(2.16)

Equation (2.15) represents the excess carrier distributions across one dimension within the sample under the assumption of a delta function optical excitation pulse (one whose duration is negligibly short with respect to carrier diffusion or recombination times). At time $t=0$, the infinite series expresses the instantaneous, steep exponential absorption profile according to Beer's law that is characteristic of the monochromatic excitation laser. As time progresses, the carrier distribution progressively diffuses and recombines into a
general distribution with surface recombination gradients. After about one effective lifetime, the carrier distribution settles into a quasi-static regime in which the only diffusion taking place is to maintain the surface gradients caused by surface recombination (i.e., "approximate homogeneity.")

In the infinite series of eqn. 2.15, each term (i.e., eigenmode) has an exponential decay coefficient of $D_p \alpha_i^2$. The effect of these decay constants is that each term decays on a vastly different time scale; the higher the mode number, the more rapid the decay of the term. For example, if the pair of surface recombination velocities are each effectively infinite, the eigenvalues $\alpha_i$ are proportional to their indices, so that the decay coefficients $D_p \alpha_i^2$ increase as $i^2$. In such a case, the highest order modes disappear so rapidly that only a few of the lowest order terms are required for an accurate representation of the majority of the time expanse of the evolving carrier distributions. Additionally, longer excitation wavelengths decrease the sharpness of the initial carrier absorption, which means that the amplitudes of the higher-order terms are relatively smaller; fewer terms are needed to adequately express the carrier distribution.

![Excess Carrier Distributions](image)

Fig. 2.5: Excess Carrier Distributions within a measurement sample at 0, $10^{-6}$, $10^{-5}$, $10^{-4}$ and $10^{-3}$ seconds after cessation of the excitation; height of the leftmost side of the curve indicates temporal priority. Bulk lifetime is $10^{-3}$ secs.; there is no surface recombination. Diffusivity is 35 cm$^2$/s, absorption coefficient is 1000 cm$^{-1}$; sample width is 300 microns. This figure is jagged because it was computed using a finite number of terms from the infinite series representation of eqn. 2.15.
As an example of the decrease of the number of series terms required as time progresses, figure 2.5 depicts a time-sequence plot of the excess carrier distributions in an undiffused (junctionless) sample with zero surface recombination occurring. The order of the terms in the time sequence is from greatest to least magnitude at the leftmost of the plot. Thirty Fourier series terms are used for the initial carrier profile, but considerable ripple is present. The second profile uses only five terms, and is completely smooth at 111000 of the bulk lifetime. Two terms are used for the third profile, three for the fourth profile, and only one term is needed for the last profile. With zero SRVs, the effective lifetime is due solely to bulk recombination, and thus, recombination is occurring at the slowest possible rate in this sample.

![Graph](image)

Fig. 2.6: A time progression of carrier profiles for infinite SRVs at both surfaces, bulk lifetime of 1 millisecond. Profiles are for time = 0, 10^{-6}, 10^{-5} seconds. Thirty, five, and one Fourier term(s) are used, respectively, which accounts for the jaggedness. Diffusivity is 35 cm^2/s; absorption coefficient is 1000/cm; sample width is 300 microns.

Figure 2.6 shows a case for infinite surface recombination velocities (i.e., zero excess carrier concentration maintained at the surfaces). The bulk lifetime is also 1 millisecond as in the previous case, but because of the large surface recombination velocities, the overall (effective) lifetime is much shorter than in the previous case. Because of this short effective lifetime, only three snapshots in the time sequence, as compared with five in the previous example, could be displayed on the vertical range chosen.
An alternative, non-Fourier series representation for the carrier distribution is possible for the somewhat restricted case of zero carrier concentrations at one surface \cite{23}. This form is an unwieldy chain of complementary error functions which \textit{occur} as a result of the convolution integral of the initial (single-exponential) photogeneration distribution with the one-dimensional Green's function for diffusion, which is a Gaussian. It is of limited usefulness for any present purposes because of its restriction, and incidentally, prove no \textit{simpler} to calculate.

2.6 Chapter Summary

The "effective" lifetime theory of contactless PCD has been presented. The result \textit{obtained} is a single number, the effective lifetime of the sample, which is a combination of the bulk lifetime, surface recombination velocities, and the diffusivity of the measurement \textit{sample}. That theory does not separate bulk and surface recombination, and relies on the fact that the photoconductive decay always asymptotically approaches a single-exponential form.

The theory for microwave detection was presented. That theory approximates the probing microwaves as plane waves and the excess carrier \textit{distributions} in the sample as \textit{varying} only along the normal axis to the broad sample surfaces. At present, microwave-detected PCD fits the reflectance decay curve in the long-time asymptotic regime, in which the carrier concentrations are approximately homogeneous within the \textit{sample}, and thus \textit{produces} only an effective lifetime.

The theory for inductively-coupled PCD was also presented. That theory described the photoconductivity of the sample as an ohmic loss across the terminals of a small \textit{detecting} coil placed plane-parallel to the sample. The detecting coil is \textit{part} of an RF bridge circuit which is imbalanced by the photoexcitation.

The general low-injection minority carrier concentrations within the equilibrating \textit{measurement} samples can be described by an infinite Fourier series solution to the boundary-value minority-carrier diffusion equation. This provides \textit{direct} insight into the carrier diffusion and recombination occurring within the sample during the initial portions of PC decay, and raises the question of the dependence of the microwave reflection on the time-varying carrier distributions in the sample, which is the subject of Chapter 3.
3. CONSIDERATION OF MICROWAVE-DETECTION PHENOMENA

3.1 Introduction

The purpose of this chapter is to discover whether the initial portion of microwave-detected PCD curves can be attributed solely to recombination in the sample. That is, it is desired to discover whether microwave-detected PCD senses the distribution of carriers in the measurement sample. Since microwave-detected PCD measures a reflectance transient and only indirectly the excess carrier transient, the relationship between the carrier distributions and the reflectance in the initial portions of the decay determine whether that part of the decay can be used as information for recombination parameter separation.

The most general causes of the rapid, initial PCD decay could be any of the following: position-detection of the carriers due to diffusion, change in bulk lifetime because of injection level, injection-level dependence of diffusivity or surface recombination velocities, time-dependent scattering of microwaves. For instance, since the excess carriers are photogenerated in a spot which is smaller than the microwave detection area, the one-dimensional carrier distribution assumption may not always be valid: some cases may require consideration of carrier diffusion and distribution parallel to sample surfaces. Also, time-dependence of the carrier distribution in the surface-parallel direction raises the possibility of a time-dependent scattering pattern of the probing microwaves, an effect that could make the measured reflectance transient different from that which would be expected from a strictly one-dimensional distribution.

At present, many authors simply ignore the early portion of the decay curve, which posed no problem since they were not pursuing what is herein being proposed. Since the purpose is to discover a method by which to separate bulk and surface recombination from PC decay, it is necessary to understand the factors causing the early portion of the decay, for more than the asymptotic decay must be utilized. Ideally, it would be convenient to show that the early portion of the PCD decay curve is due only to carrier recombination in the sample. Therefore, this chapter considers some of the phenomena associated with the microwave-detection version of PCD.
3.2 Excess Carrier Distribution Effects

To consider the dependence of microwave reflectance upon the distributions of conductivity in the measurement sample, some simple calculations are now performed. Using the plane-wave theory presented in section 2.3, some planar sheets of conductivity are now embedded at various depths within a sample. (These sheets are physically improbable, but serve as the most direct and extreme test of the sensitivity to carrier distributions of a microwave probe.)

In the following calculations, the μW-PCD wave-impedance system that is analyzed consists of four layers: an air layer, a silicon sample of 300 microns thickness, a second air layer of 0.5 cm, and a copper reflecting plate (\(a = 58,000 \, \text{S/cm}\)). (Oxide layers that are usually present on the surfaces of silicon have negligible effect upon the reflectance because of their thinness relative to the microwave probe's wavelength.) The air layers are considered lossless, with unity relative dielectric constant. The relative dielectric constant of the sample is taken as 11.7. The sample to metal plate spacing is taken as 0.5 cm for all the calculations, which results in reflectance changes of maximum sensitivity (maximum absolute slope). To simplify the calculations and aid in interpreting them, only regions of uniform conductivity are employed in the calculations.

The microwave reflectances are considered at a frequency of 9.6 GHz, (corresponding to a wavelength in vacuum of about 3.1 cm). This is the frequency used by many experimenters (and which will be used for this study), but the use of higher frequencies is not uncommon.

3.2.1 Sensitivity to carrier distributions normal to surfaces

The reflectivity of a sample for depth-insensitive probes is determined only by the total number of excess carriers, and does not in any way depend upon their distribution within the sample. In this section, a simple test of sensitivity to carriers distributions of a microwave probe will be described.

Figure 2.3 depicted a reflectance function versus conductivity for a four-layer system of air/wafer/air/reflecting plate. However, points on that curve were for nonexcited, homogeneously conductive samples (no carrier distributions). In excited samples in the early stages of carrier decay, the conductivity is not homogeneous, so that a depth-sensitive PCD reflectance would not lie on a point on the curve, nor would a PCD curve trace out a portion of the reflectance curve. Thus, it is possible that bulk carrier diffusion within samples may introduce a time-constant into the reflectance versus conductivity function, depending on the microwave frequency that is used.
To investigate the ability of the $\mu$W-PCD technique to sense variations in conductivity along the direction normal to the sample surfaces, reflectances were computed for a series of samples having equal sheet conductances, but with each differently distributed. The excess conductivity of each layer was scaled by its thickness so that each sample possessed an equal excess sheet conductance.

By comparing the reflectances of these samples, an elementary test of the technique's ability to sense carrier depth distributions is obtained. Since the regime of maximum sensitivity to changes in reflectance occurs for conductivities on either side of the minimum in figure 2.3 (the region of greatest absolute slope), the equilibrium conductivities of the samples were taken in this range so as to test the most sensitive cases. For this reason, the reflectance results presented show maximal differences in carrier distribution, and are the limiting cases for this type of sensitivity.

![Diagram of sample layers](image)

**Fig. 3.1:** Excess conductive layer positions within a sample.

Table 3.1 compares the reflectances of samples with equilibrium conductivities of $0.02$ Siemens/cm (about $2 \times 10^{14}$ p-type doping). The layer of excess conductivity in each sample has the same radius as the sample, varying thickness, and is located within the sample in one of the locations diagrammed in figure 3.1. Although the layers are quite different in location and/or conductivity, the difference in reflectances among the samples is less than 3 parts in 100.
Table 3.1
Reflectances of equilibrium samples with added single plane conductive layers. Left column gives the conductivity, thickness, and location of the layer (see fig. 3.1). Equilibrium conductivity of each sample is 0.02 S/cm; the overall sheet conductances of each sample are equal.

<table>
<thead>
<tr>
<th>Layer Description</th>
<th>Reflectance</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.2 S/cm, 300 microns</td>
<td>0.3062</td>
</tr>
<tr>
<td>0.6 S/cm, 100 microns, near surface</td>
<td>0.3119</td>
</tr>
<tr>
<td>0.6 S/cm, 100 microns, center</td>
<td>0.3014</td>
</tr>
<tr>
<td>0.6 S/cm, 100 microns, far surface</td>
<td>0.2949</td>
</tr>
<tr>
<td>2.0 S/cm, 30 microns, near surface</td>
<td>0.3133</td>
</tr>
<tr>
<td>2.0 S/cm, 30 microns, center</td>
<td>0.3012</td>
</tr>
<tr>
<td>2.0 S/cm, 30 microns, far surface</td>
<td>0.2916</td>
</tr>
</tbody>
</table>

Table 3.2:
Reflectance of equilibrium samples with added planar conductive layers. Left column gives the conductivity, thickness, and location of the layer (see fig. 3.1). Equilibrium conductivity of each sample is 0.2 S/cm; the overall sheet conductances of each sample are equal.

<table>
<thead>
<tr>
<th>Layer Description</th>
<th>Reflectance</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.2 S/cm, 300 microns</td>
<td>0.5266</td>
</tr>
<tr>
<td>0.6 S/cm, 100 microns, near surface</td>
<td>0.5298</td>
</tr>
<tr>
<td>0.6 S/cm, 100 microns, center</td>
<td>0.5254</td>
</tr>
<tr>
<td>0.6 S/cm, 100 microns, far surface</td>
<td>0.5220</td>
</tr>
<tr>
<td>2.0 S/cm, 30 microns, near surface</td>
<td>0.5308</td>
</tr>
<tr>
<td>2.0 S/cm, 30 microns, center</td>
<td>0.5254</td>
</tr>
<tr>
<td>2.0 S/cm, 30 microns, far surface</td>
<td>0.5204</td>
</tr>
</tbody>
</table>
Table 3.2 displays the results for samples with 0.2 S/cm background conductivity. As was true in table 3.1, the reflectances are very similar, differing at most by a little over 1 part in 100.

3.2.2 Lateral carrier diffusion

This section considers the diffusion of carriers parallel with the sample surfaces. This second dimension of carrier action is of interest because it may undesirably contribute to the shape of the early portion of the PCD decay curve. It is relevant for those who are using PCD apparatuses to map localized carrier lifetimes across the breadth of samples and are therefore employing an excitation beam which may be equal or smaller in spot size than the microwave detection beam coverage. With such a configuration, there is a question as to the accuracy of the generally accepted 1-dimensional carrier-distribution theory, owing to the inherently 2-dimensional diffusion (lateral as well as longitudinal) of carriers under such excitation.

Since the actual excitation laser spot and absorption pattern are cylindrically symmetric, the minority carrier diffusion equation in two dimensions \((\rho, z)\) can be solved by the method of separation of variables \([28]\). Its solution is the product of the independent \(z\) component distribution (previously given in eqn. 2.15) and cylindrical distribution.

The cylindrical distribution can be found by assuming that the excitation laser's intensity profile is Gaussian, and convolving it with the Green's function for carrier diffusion \([29]\) (which is also Gaussian). This result assumes that the excitation spot is far from the wafer edges.

\[
\Delta p(\rho, t) = \frac{\Delta p_0}{2\Lambda^2} \exp \left[ -\frac{\rho^2}{2\Lambda^2} \right]
\]

where

\[
\Lambda = \sqrt{a^2 + \left(\frac{2D_p t}{a^2}\right)^2}
\]

is the lateral carrier distribution radius. It can be seen that the initial, \(t=0\) distribution radius equals \(a_0\), the excitation spot size, and that the radius diverges in the limit of infinite time. The radial size of the distribution will not expand until \(2D_p t\) becomes appreciable to \(a^2\). Since \(\Lambda^2 = a^2(1 + 2D_p t/a^2)\), \(a^2/2D_p\) is the time constant of the radial distribution. If this time constant is small compared with the effective lifetime of the sample, the approximation
that the distribution is solely one-dimensional proves to be accurate. (However, this is apart from considerations of time-dependent microwave scattering from the radially inhomogeneous conductivity distribution.)

For most highly absorbed sources, the radial carrier gradients will be much shallower than those in the $z$ (longitudinal) direction, but it is still possible that lateral (radial) diffusion may play a role in modifying the detected carrier decay rate. This is because the carrier density in the center (detected) area of the distribution might decrease in amplitude because of lateral diffusion on the same time scale as does recombination. In such a case, because of the product form of the two-dimensional carrier distribution the amplitude of the excess carrier distributions will decay more rapidly than what the one-dimensional theory would predict, resulting in an "artificially" foreshortened PCD decay, and therefore, a shortened effective lifetime. If appreciable loss of carrier density is occurring at the center of the detection area, it is conceivable that this unaccounted-for lateral carrier decay would result in artificially low lifetime readings.

3.2.3 Reflectance dependence upon diffusion parallel to surfaces

As was seen in the above section, carriers are non-uniformly generated on the face of measurement samples (i.e., in a spot). Therefore, in general, it is expected that these carriers will have a component of diffusion parallel with the sample surfaces. Since the thickness of the sample is considerably less than the diameter of the sample, diffusion normal to the surfaces should cease much more rapidly than in the surface-parallel direction.

Might the surface-parallel diffusion component have an effect on the reflectance decay transient, since the generation spot size is smaller than the area covered by impinging microwaves? To explore the answer to this question, a first-order calculation of the dependence of reflectance upon post-excitation excess carrier spot size was carried out by computing the reflectance of a sample as the area-weighted average of its background conductivity plus the reflectance of a series of different-sized embedded disks of excess conductivity. For purposes of comparison, the conductivity times area of the embedded disks was held constant across a series, so that larger disks were of less conductivity per unit area than the smaller disks.

In terms of the $\mu$W-PCD technique, the reflectances of a sample with a series of embedded disks of increasing area roughly corresponds to the reflectances of a sample at specific instants of time for the idealized case of surface-parallel diffusion so rapid that no carriers recombine. ("Roughly" means that carrier mobility was held constant, regardless of
carrier concentration.) Admittedly, this is quite idealized, since it assumes that an excitation spot can have surface-parallel diffusion this drastic; however, its purpose it to demonstrate the worst-case effect that an increasing conductivity spot may have upon a measured decay.

Figure 3.2 below depicts the embedded disk areas employed in the study as percentages of the total sample area occupied.

![Relative disk areas for the surface-parallel diffusion study](image)

**Fig. 3.2:** Relative disk areas for the surface-parallel diffusion study, (areas are to scale).

Consider figure 2.3 again. Under the one-dimensional theory, as long as the sample conductivity (excess plus background) does not cross the minimum, the result should be a monotonic decay. For background conductivities to the left of the minimum, a decaying excess conductivity should always result in a monotonically increasing reflectance. When the background conductivity is to the right of the minimum, any excess conductivity decay should always result in a monotonically decreasing reflectance. The studies below consider what occurs if surface-parallel diffusion might cause an area-weighted reflectance effect.

Table 3.3 shows computed reflectances when the background conductivity of the sample is to the left of the minimum in figure 2.3. The table reveals that considerable differences in reflectance are possible depending upon the embedded disk area. Per the above discussion, scanning the reflectances from left to right across a row of table 3.3 shows an idealized time-dependent reflectance trend caused by surface-parallel diffusion. In
some instances, the change in reflectance is opposite to that which is caused by carrier recombination (decrease in conductivity). Normal conductivity decay transients to the left of the minimum should cause increases in reflectance; however, for cases when the disk size may change appreciably during the decay, non-monotonic transients might occur. In addition, row 3 also contains a non-monotonic reflection transient (between the 50% and 100% columns) caused because the "100%" disk's excess conductivity causes it to be to the right of the minimum in figure 2.3.

Table 3.3
Area-weighted reflectance of a sample (background conductivity = 0.02 S/cm) when conductive disks of various areas are embedded in it. (Top row shows the percentage of the total sample area occupied by the embedded disk; the left-most column shows the excess conductivity of the embedded disk when it is the same size as the sample.)

<table>
<thead>
<tr>
<th>S/cm</th>
<th>5%</th>
<th>10%</th>
<th>20%</th>
<th>50%</th>
<th>100%</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.02</td>
<td>0.3324</td>
<td>0.3198</td>
<td>0.2778</td>
<td>0.1757</td>
<td>0.0931</td>
</tr>
<tr>
<td>0.01</td>
<td>0.3205</td>
<td>0.2996</td>
<td>0.2623</td>
<td>0.2072</td>
<td>0.1758</td>
</tr>
<tr>
<td>0.2</td>
<td>0.3517</td>
<td>0.3769</td>
<td>0.4125</td>
<td>0.4322</td>
<td>0.3062</td>
</tr>
</tbody>
</table>

Table 3.4
Area-weighted reflectance of a sample (background conductivity = 0.2 S/cm) when conductive disks of various areas are embedded in it. (Top row shows the percentage of the total sample area occupied by the embedded disk; the left-most column shows the excess conductivity of the embedded disk when it is the same size as the sample.)

<table>
<thead>
<tr>
<th>S/cm</th>
<th>5%</th>
<th>10%</th>
<th>20%</th>
<th>50%</th>
<th>100%</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.02</td>
<td>0.2896</td>
<td>0.2961</td>
<td>0.3011</td>
<td>0.3048</td>
<td>0.3062</td>
</tr>
<tr>
<td>0.01</td>
<td>0.2833</td>
<td>0.2858</td>
<td>0.2873</td>
<td>0.2884</td>
<td>0.2887</td>
</tr>
<tr>
<td>0.2</td>
<td>0.3036</td>
<td>0.3321</td>
<td>0.3778</td>
<td>0.4617</td>
<td>0.5266</td>
</tr>
</tbody>
</table>

Table 3.4 compares reflectances for a sample whose equilibrium conductivity is to the right of the minimum in figure 2.3; every excess conductivity transient in those conductivity ranges should produce decreases in reflectance. Table 3.4 demonstrates that a conductive area which is increasing in size can change the reflectance transient in a direction opposite to that which recombination does. (The effect in table 3.4 is not as pronounced as
in table 3.3 because the added conductivities are smaller percentages of the sample's background conductivities.)

3.2.4 Time-dependent microwave scattering

The previous section considered the dependence of the reflectance decay strictly due to carrier diffusion and the changes in carrier density that result. In this section, the effect of time-dependent microwave backscattering is the subject of interest. Here, the distinction is being made between perfect, planar microwave reflection and the possibility of a time-dependent scattering pattern that could occur because of the size and shape of the excitation spot created in the measurement sample. Any scattering pattern, if not time-dependent, is of no consequence, since it would only scale the amplitude of the reflectance transient. However, if the scattering amplitude on the detector axis was to vary during the transient, this variation in the amplitude of reflected microwaves reaching the detector would introduce an additional, unwanted time constant into μW-PCD results.

To investigate the possibility of this time-dependent scattering, the excess carrier distributions parallel to the sample surfaces were again modeled as disk-shaped regions on whose broad face the microwaves were normally incident. The disk is a geometrical shape that has a closed form solution for its polar amplitude scattering pattern when considered under the Born approximation of scattering theory [27]; that solution is

\[ F(\theta_0) = \frac{2J_1(ka \sin \theta_0) \sin \left( \frac{kd (\sin \theta_0)^2}{2} \right)}{kd (\sin \theta_0)^2}, \]

where \( J_1 \) is the Bessel function of the first kind, order 1, "a" is disk radius, "d" is disk thickness, "k" is the wave number in the region exterior to the disk, and \( \theta_0 \) is the polar scattering angle. \( \theta_0 = 0 \) degrees is the axis normal to the broad surface of the disk.

To consider the time-dependence of microwave scattering, the scattering patterns for a sequence of disks of increasing size would ordinarily be computed. However, as will be shown, the dimensions of the disk relative to the wavenumber of the probing microwaves are such that the scattering pattern is isotropic except for maximum disk sizes that could be seen in silicon. Therefore, the scattering pattern for the maximum disk size is plotted and the shape of patterns for the smaller disks is described relative to it.

The scattering pattern of eqn. 3.3 is plotted in figure 3.3 for the conditions given below (for a maximum disk size). The left horizontal axis of the figure is the direction of
incident microwaves \((\theta_0 = 0\) degrees). The disk thickness was taken as 300 microns (corresponding to the thickness of a nominal sample), and its radius was taken as 0.4 cm., which roughly corresponds to 2 electron diffusion lengths in a high-quality intrinsic silicon sample (diffusivity of 35 \(\text{cm}^2/\text{s}\) and a bulk lifetime of 1 millisecond). The exterior wavenumber was computed for a wavelength of 3.1 cm (a 9.6 \(\text{GHz}\) microwave frequency in air). The pattern is nearly isotropic, with the relative scattering larger along the zero degree axis.

![Polar scattering of 9.6 GHz microwaves normally incident on the face of a disk-shaped conducting region, 300 \(\mu\text{m}\) thick, with radius 0.4 cm. Surrounding medium is air.](image)

The scattering function in eqn. 3.3 is the product of two quotients which are each a maximum when their arguments are zero (see figures 3.4 and 3.5 below). Because of the shape of these quotient functions and the value of the parameters used for the plot of figure 3.3, it is unnecessary to plot the scattering function for smaller disks, since these are necessarily more isotropic. The scattering pattern in figure 3.3 has \(k \alpha = 0.8\), which becomes smaller for smaller disks, and therefore increases the value of the first quotient function towards unity (plotted in figure 3.4) for all angles. Any disk (sample) thicknesses within reason have little or no bearing on the scattering pattern since they are insignificant relative to the probing wavelength \((k\!d = 0.06\) was used in figure 3.3, and the effect of this disk
dimension can be seen in figure 3.4). Therefore, smaller disk radii than that used in figure 3.3 produce more nearly isotropic scattering patterns. Therefore, the slight anisotropy of figure 3.3 means that a slightly larger percentage of incident microwaves may be back-scattered toward the detector at the end of a transient decay (that is, when surface-parallel carrier distributions reach their maximum extent), but this would occur only in samples with very large diffusion lengths.

![Graph of eqn. 3.3](image)

Fig. 3.4: Plot of the first quotient term in the polar scattering function of eqn. 3.3.

It appears that very little time-dependence of scattering will occur for the majority of silicon samples at low microwave frequencies. However, if measurements are made on materials with greater diffusion lengths, or are made on silicon using higher microwave frequencies, time-dependent scattering might become an important issue affecting measured PCD decays.
3.3 Summary of Results

In this chapter, the major phenomena that might have had an effect upon microwave-detected PCD curves were considered. The studies showed that at low microwave frequencies, carrier depth distributions are not sensed in measurement samples. Therefore, there is no depth sensitivity, so that carrier diffusion normal to the sample surfaces does not contribute to the shape of the PCD decay curve.

The effect of finite excitation spot-size upon microwave reflection was also considered. The derived analytical expression showed that if the spot-size is chosen large enough, no lateral spreading of carriers can occur within the time-frame of the other decay time-constants in the sample.

Other studies considered the dependence of reflectance upon two superimposed areas of conductivity, such as an excitation spot and its surrounding non-excited area. It was shown that this could have a large effect upon the overall reflectance; however, if as above, the spot-size is chosen large enough, there is negligible change in the lateral carrier distributions on the time scale of the recombination in the sample, and therefore, this area effect can be negated.
Lastly, the effect of scattering upon the microwave reflectance was considered. However, as above, if the spot-size is chosen judiciously, since the conductive area does not vary appreciably, no time-dependence of scattering can occur.

Therefore, the net effect of general carrier distributions (created by a monochromatic excitation beam of finite spot size) upon the microwave reflectance of such samples can be negated through the use of sufficiently low-frequency microwaves, and a sufficiently large excitation spot-size. *For this reason, the microwave detection can be configured to be independent of all effects but recombination in the measurement sample.*
This page intentionally left blank.
4. STUDY OF EQUATION COMPONENTS FOR THE PURPOSES OF RECOMBINATION PARAMETER SEPARATION

4.1 Introduction

Since the PCD probes being considered do not sense carrier position nor diffusive carrier motion within the sample, the PCD theory can be specialized for these cases. This specialization consists of integrating the minority carrier distribution expressions across the measurement sample, which eliminates all carrier position dependence in the theory. This integration simplifies the PCD theory in a beneficial way for the present purposes. The consequences of this simplification and their impact on the ability to separate recombination parameters are the subject of this chapter. The theory presented in this chapter is more general than that presented by some authors ([5], for example), in that it considers two different surface recombination velocities.

4.2 Depth-Insensitive PCD Theory, Generalized for Two Independent Surface Recombination Velocities

The following theory can be constructed for the PCD technique, assuming that a depth-insensitive probe is employed under low-level carrier injection conditions. To obtain the total carrier concentrations, the carrier distributions in the sample must first be obtained. Assuming that diffusivity and surface recombinations are constant, and that the excitation is a delta-function of time, the minority carrier distributions in the sample are expressible as an infinite Fourier series (derived in Appendix A)

\[
\Delta p(x,t) = \sum_{i=1}^{\infty} A_i e^{-k_i} \left[ \cos(\alpha_i x) + \frac{S_i}{\alpha_i D_p} \sin(\alpha_i x) \right]
\]

where the parameters will be defined below. Because of insensitivity to carrier distribution, only the total number of excess carriers in the sample are detected by the PCD probes under
consideration. In addition, because of the ability to vary the linearity of the sample's reflectance versus conductivity characteristic, and because at low-injection levels carrier mobilities remain constant, every other aspect of the measurement chain contributes only a multiplicative constant to the total excess carriers in the sample. Thus, the expression for the measured microwave reflectance can be made to be a constant times the total number of excess carriers in the sample. Integrating eqn. 4.1 across the spatial dimension (and multiplying by the undetermined system constant) yields the desired result, the expression for the total excess carriers in the sample. Therefore, the form of the PCD decay curve is an infinite series of decaying exponentials, each having its own amplitude and decay constant,

$$S(t) = C_{\text{system}} \int_{x=0}^{x=W} \Delta p(x,t) \, dx = C_{\text{system}} \sum_{i=1}^{\infty} C_i e^{-k_i t}.$$  

Because of this, depth-insensitive PCD data can be decomposed by finding the amplitudes $C_i$ and decay coefficients $k_i$ of its constituent terms. (The unique case in which both surface recombination velocities are zero results in a total carrier concentration expressed as a single term, which is a constant times an exponential that decays as the inverse bulk lifetime [28].)

4.2.1 Exponential decay coefficients

Consider the parameters in eqn. 4.2. The exponential decay coefficients $k_i$ are each the sum of a surface recombination velocity (SRV) dependent term and the inverse bulk lifetime; that is,

$$k_i = D_p \alpha_i^2 + 1/\tau_b$$

where $\tau_b$ is the bulk lifetime of the sample, and $1/D_p \alpha_i^2$ (often called the surface lifetime) is a term that depends upon the sample's thickness $W$, diffusivity $D_p$, and both of its surface recombination velocities.

4.2.2 Decay eigenvalues

The carrier distribution eigenvalues $\alpha_i$ in eqn. 4.3 are an important factor in the decay coefficients $k_i$ and the term amplitudes $C_i$. Therefore, it is beneficial to consider them in detail, since any strategy for separating bulk and surface recombination must include a method for finding the SRVs from these eigenvalues.
The $\alpha_i$ are the solutions to the transcendental eqn 4.4 involving diffusivity, the SRVs, and sample thickness, $W$.

$$\tan(\alpha_i W) = \frac{\frac{\alpha_i}{D_p}(S_1 + S_2)}{\left(\alpha_i^2 - \frac{S_1S_2}{D_p^2}\right)}.$$  \hfill (4.4)

$S_1$ is the surface recombination velocity (SRV) at the excited surface, and $S_2$ is the SRV at the opposing surface. (References [5] and [8] contain more information about the eigenvalues and distributions, although they consider only the case $S_1 = S_2$.)

For this study, it is more convenient to work with the following normalized variables: $a_i = \alpha_i W$, and $b_i = S_i W / D_p$. (Henceforth, the $a_i$ will be referred to as eigenvalues and the $b_i$ will be referred to as SRVs with the understanding that these are normalized parameters.) This normalization reduces the number of independent variables, thus making it easier to carry out exhaustive studies of the effects of variations in their values. This normalization changes eqn. 4.4 into

$$\tan(a_i) = \frac{a_i(b_1 + b_2)}{(a_i^2 - b_1b_2)}.$$  \hfill (4.5)

To further simplify this study, consider a reformulation of the surface recombination velocities. Observe that eqn. 4.5 is symmetric in the surface recombination velocities (exchange one for the other, leaving the equation invariant). Therefore, it is perfectly valid to express the SRVs in terms of their average and half their difference; that is, define $\bar{b} = (b_1 + b_2) / 2$ and $\Delta b = \max\{b_1, b_2\} - \bar{b}$, where $\Delta b$ is restricted to the range $[0, \bar{b}]$. This formulation makes eqn. 4.5 to be

$$\tan(a_i) = \frac{2a_i\bar{b}}{a_i^2 - \bar{b}^2 + \Delta b^2}.$$  \hfill (4.6)

From this form, several useful facts can be ascertained. First, for a fixed $\bar{b}$, the maximum value of the right hand side occurs when $\Delta b$ is a minimum value (zero). Thus, for a given $\bar{b}$, $a_i$ is a maximum when the surface recombination velocities are equal. Conversely, for a
for a fixed $\bar{b}$, $a_i$ is a minimum when $\Delta b$ is its maximum value of $6$; that is, when one SRV is $2\bar{b}$ and the other is zero.

For a fixed $\bar{b}$, it can be shown that the maximum spread of values of $a_i$ is $\pi/2$ as $A\bar{b}$ varies. This occurs when $\bar{b}$ is very large and $\Delta b$ is as much as $\bar{b}$. In most cases, the range of variation with $\Delta b$ is much smaller. Another important fact is that each of the eigenvalues $a_i$ is monotonic in $\bar{b}$, as can be seen in figure 4.1. In addition, each $a_i$ lies exclusively within its own interval $(i-1)\pi$ and $i\pi$, where $i$ is an integer in the range $[1, \infty)$.

Fig. 4.1: Normalized eigenvalues (indices=1,2,3) vs. the base-10 logarithm of surface recombination velocity for $W=400$ microns, $D=20$ cm$^2$/sec.

Considering eqn. 4.6 again, it can be seen that since the "starting point" (SRVs=0) of each $a_i$ is a multiple of $\pi$, the increase of $\bar{b}$ does not take effect on the right member of each equation as rapidly for the higher-index equations as for lower-order equations. This accounts for the different curve shapes in figure 4.1. Because of this, the eigenvalues are not in general harmonically related. (A great practical simplification in the calculations and theory would occur if this were to have been true.)
4.2.3 Term amplitudes

The form of the carrier distribution amplitudes $A_i$ and the microwave reflectance amplitudes $C_{\text{system}}C_i$ depend upon the initial carrier distributions, which, for a monochromatic (e.g., laser diode) excitation source is given approximately by Beer's law (exponential decay with distance into the sample), and are

$$A_i = \frac{n_1}{\text{denom}}$$

and

$$C_{\text{system}}C_i = C_{\text{system}}A_i \ast n_2 = C_{\text{system}} \frac{n_1 \ast n_2}{\text{denom}}$$

where

$$n_1 = \frac{\gamma F \left\{ \left( \gamma + \frac{S_i}{D_p} \right)(1 - e^{-\alpha_i W}) + e^{-\alpha_i W} \left[ \alpha_i - (\gamma S_i) / (\alpha_i D_p) \right] \sin(\alpha_i W) \right\}}{\left( \gamma^2 + \alpha_i^2 \right)}$$

$$\text{denom} = \frac{1}{2 \alpha_i^2} \left\{ \left( \frac{S_i}{D_p} \right) \left[ \frac{\alpha_i^2 + \left( \frac{S_i}{D_p} \right)^2}{\alpha_i^2 + \left( \frac{S_i}{D_p} \right)^2} \right] + \left( \frac{S_i}{D_p} \right) + \left[ \alpha_i^2 + \left( \frac{S_i}{D_p} \right)^2 \right] \right\}$$

and

$$n_2 = \frac{1}{\alpha_i^2} \left\{ \left( \frac{S_i}{D_p} \right)(1 - \cos(\alpha_i W)) + \alpha_i \sin(\alpha_i W) \right\}.$$
signal, the $k_i$ and the $C_{\text{system} i}$, were known, would these lead back to a unique set of the recombination parameters? Since any separation strategy must proceed backwards from the PCD curve to the recombination parameters that caused them, it is required that the PCD parameter functions have unique inverses. That is, it is required that the functions be monotonic in the recombination parameters. The properties of combinations of the PCD parameters will be considered in this section for the purpose of discovering if they have the required properties.

### 4.3.1 Differences between adjacent eigenvalues

The difference between adjacent eigenvalues $a_i$ as a function of $\bar{b}$ is plotted in figure 4.2.

![Fig. 4.2: Eigenvalue spacings vs. S (where S1=S2=S); W=400 microns, D=20 cm²/sec.](image)

These differences are obviously not a monotonic function of $\bar{b}$. Recall that the $i$-th eigenvalue occurs in its own partition of $[(i-1)\pi, i\pi]$, and therefore although the left hand side of eqn. 4.5 is periodic, the right hand side is not. Thus, the regime in which $\delta$ and $\Delta b$ begin to affect the respective eigenvalues comes at larger SRVs as $i$ increases, causing eigenvalue differences $a_j - a_i, j \neq i$ to be non-monotonic. Therefore, a fixed value of this
difference does not uniquely define a pair of \((S_1, S_2)\), and is therefore valueless for the present purpose.

4.3.2 Differences of squared eigenvalues

Figure 4.3 shows the squared differences between adjacent eigenvalues, \(a_j^2 - a_i^2, j = i + 1\).

![Graph showing squared eigenvalue differences](image)

Fig. 4.3: Squared eigenvalue differences \(a_j^2 - a_i^2, j = i + 1\) (for \(i=0,1,2,3\)) vs. \(S\); \(W=400\) microns, \(D=20\) cm\(^2\) sec.

It can be seen that these differences are monotonic (although only mildly so for small SRVs.) This is particularly helpful because the difference \(k_j - k_i, j \neq i\) is proportional to \(a_j^2 - a_i^2\), and is also independent of the bulk lifetime.

As mentioned above, the eigenvalues are limited to ranges which are subsequent integer multiples of \(\delta\). Thus, in addition, the maximum and minimum difference between decay coefficients \(k_j - k_i, j \neq i\) is well-defined. For instance, the minimum value of \(a_1\) is zero, while the minimum value of \(a_2\) is \(\pi\). Likewise, their respective maximum values are \(\pi\) and \(2\delta\). Therefore, \(a_2^2 - a_1^2\) must fall in the range \([\pi^2, 3\pi^2]\). This is of practical utility in that one may take \(k_2 - k_1\) and calculate the possible range of diffusivities that might have occurred, that is,
so that

\[ \frac{W^2}{D_p} (k_2 - k_1) = (\alpha_2^2 - \alpha_1^2) \]  

must fall in the range \([n^2, 3n^2]\), which sets the range of possible diffusivities for any particular results extracted from a data set (assuming that the sample thickness can be accurately measured.)

Figure 4.4 shows the full surface for \(k_2 - k_1\) (two independent SRVs.) It is monotonic along any line which is parallel to the main floor diagonal, and is also symmetric in the SRVs.

Fig. 4.4: A plot of the normalized difference between second and first decay coefficients \(W^2(k_2 - k_1)/D_p = (\alpha_2^2 - \alpha_1^2)W^2\) versus \(\{s_1, s_2\}\) for \(W = 400\mu m\) and \(D_p = 12.8 cm^2/sec\).
4.3.3 Ratio of second and first amplitudes

The amplitudes $C_i$ are large, complicated expressions (eqns. 4.8-4.11). However, from their form it can be seen that the ratio of any two of them is independent of the system constant $C_{\text{system}}$ and the bulk lifetime, which are both of considerable practical value. Therefore, now consider the ratios in more detail. Figure 4.5 depicts the ratio $C_2/C_1$ for the absorption coefficient of a GaAs laser diode, 294/cm. It can be seen this ratio is highly asymmetric in the SRVs, which is due to the highly-absorbed (depthwise asymmetric) profile of the excitation source (recall that the Fourier series amplitudes are fit to the initial condition, which in this case is the Beer's law distribution for the supposed monochromatic excitation source.) This asymmetry of $C_2/C_1$ with respect to the SRVs, coupled with the symmetry of $k_2 - k_1$ with respect to the SRVs, provides an interesting result, which will be discussed in the next section.

Fig. 4.5: The amplitude ratio surface $C_2/C_1$ vs. the SRVs, using the values $W = 400\,\mu m$, $D_p = 12.8\,cm^2/sec$, and $\gamma = 294/\,cm$. 
Figure 4.6 shows the analogous surface for an absorption coefficient of $11.8/\text{cm}$ (1.064 micron wavelength, the infrared line of a Nd:YAG laser.) Since this beam is so mildly absorbed that the negative values that appeared to the right of figure 4.5 have been converted into positive values. This result is a consequence of losing the high spatial asymmetry of the highly-absorbed beam, which yields larger high-order modes.

Figure 4.7 below is a third $C_2/C_1$ plot using an absorption coefficient of 7000, which corresponds to the green Nd:YAG laser line at 532 nanometers. The high absorption of this beam gives it an appearance like that of figure 4.5, only more extreme since it has greater absorption.

Fig. 4.6: The amplitude ratio surface $C_2/C_1$ vs. the SRVs, using the values $W = 400\mu\text{m}$, $D_p = 12.8\text{cm}^2/\text{sec}$, and $\gamma = 11.8/\text{cm}$. 
4.3.4 The combination of $C_2/C_1$ with $k_2 - k_1$.

Figures 4.8 and 4.9 below show the level curves for figs. 4.4 and 4.5, respectively. The latter figures are the surfaces for two independent surface recombination velocities, so that the former are, also.

In figure 4.8, the set of possible solutions $\{S_1, S_2\}$ for a particular measurement lie on the curve of intersection of a horizontal plane with the surface. Because of the even symmetry of the surface with respect to the SRVs, the level curve of possible solutions $\{S_1, S_2\}$ is always symmetric with respect to the SRVs. (Imagine a vertical plane extending from the near corner to the far corner of the figure; all level curves are mirror images about this vertical plane when viewed from above.) In figure 4.9, the possible solutions $\{S_1, S_2\}$ for a certain measurement also lie on the intersection of a horizontal plane with the surface. Because of the asymmetry of the surface with respect to the SRVs, the level curves never cross the vertical plane from the front corner to the rear corner of the figure. Therefore, overlaying the particular level curves $C_2/C_1$ and $k_2 - k_1$ for a particular sample shows that their crossing point is either unique or nonexistent (the latter case occurring if the value of...
diffusivity, which is the coefficient of \( k_a - k_1 \), is improperly chosen.) Thus, for a properly chosen value of diffusivity, the solution \( \{S_1, S_2\} \) should be unique, although there may be regimes in which sensitivity to the exact solution may be poor. The same result holds true for the combination of figs. 4.4 and 4.7; however, it is not true for some values appearing in figure 4.6, since the ratios less than the top of the right peak of the figure may appear in two places. However, the fortuitous result for highly absorbed beams is that two functions of the SRVs can be formed that are independent of all system parameters and bulk lifetime, which permit a unique solution for the two independent SRVs in spite of the fact that both functions are quite nonlinear. For less highly absorbed beams, a bi-unique solution (SRVs can be found, but not identified) can be found.

![Figure 4.8: Some representative level curves of \( k_2 - k_1 \) from fig. 4.4.](image)
4.4 Conclusion

In view of the above, recall that this is a problem in three physical parameters (unknowns) for which a unique solution is sought. (It is assumed that sample thickness can be accurately measured.) However, the properties and form of the functions $C_2/C_1$ and $k_2 - k_1$ allow the elimination of the bulk lifetime from initial consideration, isolating the two surface recombination velocities. Therefore, an algorithm for the separation of the surface and bulk recombinations can proceed by self-consistently solving for the pair of unique surface recombination velocities, then back-calculating the bulk lifetime from any of the decay coefficients $k_i$. This is the strategy that will be pursued for the separation algorithm, which is discussed in chapter 5.
5. SEPARATION ALGORITHM

5.1 Introduction

On the basis of the insights gained in chapter 4, an algorithm for obtaining distinct values for the bulk lifetime and the two surface recombinations from a single PCD curve will be presented. Since a long-wavelength probe is employed, the PCD decay curve is proportional to the total carrier concentration, which is an infinite series of decaying exponentials. In addition, the ability to linearize the other effects of the detection system enable the detected PCD signal to also be linearly proportional to the series of decaying exponentials. This supposition forms the basis of the strategy for separating surface recombination and bulk lifetime, a scheme in which the parameters of the lowest few terms are extracted from the measurement curve and the recombination parameters back-calculated from them.

Intuition would seem to suggest that the depth-insensitivity of the probe implies that no distinction of surface and bulk separation should be possible. This is generally true. However, it turns out that the mathematical form of the reflectance that results from this depth-insensitivity readily lends itself to a computational method of separation. To separate the recombination parameters (RPs) will require that the collective set of PCD decay parameters can produce a unique set of RPs when a suitable algorithm is applied to them. Failing this, it is hoped that a less desirable, but still useful set of recombination values may still be obtained (for instance, some effective surface recombination velocity value, rather than unique values for each of the surfaces).

5.2: Reasoning Behind the Algorithm

Under proper conditions (discussed in Appendix A), the form of the measured PCD curve is

\[ S(t) = C_{\text{system}} \int_{x=0}^{x=W} \Delta p(x,t)dx = C_{\text{system}} \sum_{i=1}^{\infty} C_i e^{-k't} \]  

(5.1)
In eqn. 5.1, the exponential decay coefficients $k_i$ are each the sum of a surface recombination velocity (SRV) dependent term and the inverse bulk lifetime:

$$k_i = D_p \alpha_i^2 + 1/\tau_b.$$  \hspace{1cm} (5.2)

From chapter 4, it is known that the difference

$$\delta = k_2 - k_1 = D_p (\alpha_2^2 - \alpha_1^2)$$  \hspace{1cm} (5.3)

is independent of bulk lifetime $\tau_b$, and is symmetric in the SRVs. We also know that the ratio

$$\rho = \left(\frac{C_{\text{system}}}{C_2}\right) / \left(\frac{C_{\text{system}}}{C_1}\right) = C_2/C_1$$  \hspace{1cm} (5.4)

is also independent of bulk lifetime, and is asymmetric in the SRVs. (This ratio is also independent of the photon flux of the exciter, as well as the system constant $C_{\text{system}}$ that includes factors such as the detector amplification, carrier mobilities, and the slope of the reflectance with respect to conductivity.) The properties of the amplitude ratio $\rho$ and the decay coefficient difference $\delta$ simplify the overall problem to that of finding two SRVs rather than all three unknowns at once.

5.3 The Recombination Parameter Separation Process

5.3.1 Extraction of the decay parameters from the PCD curve

The algorithm begins as follows. Assuming the infinite-series expression (eqn. 5.1) for the microwave reflectance data, the decay coefficients $k_i$ for $i=1, 2, \text{ and } 3$ are extracted from a PCD curve using the ESPRIT method (see Appendix B), executed as a script file in the commercial linear algebra package MATLAB. Knowing the $k_i$, the amplitudes $C_i$ for the same three terms are found through a least squares fit. The parameters of the $i=3$ term are then discarded; their sole purpose is to (approximately) account for the information represented by terms $i \rightarrow [3, \infty)$ thereby making the extracted $i=1$ and 2 parameters more accurate.

5.3.2 Deduction of the recombination parameters

With the PCD decay parameters in possession, the next step is to solve for the recombination parameters. The decay parameters $C_2$, $C_1$, $k_2$, $k_1$, the sample thickness $W$,
the absorption coefficient of the exciter beam, and the minority carrier diffusivity $D_p$ are input to a C language computer program for computations. The quotient $\rho = C_1 / C_2$ is taken of the second and first amplitudes, and the difference $6 = (k_2 - k_1)$ of the second and first decay coefficients is also formed. An iterative routine (see the following section) then searches for the pair $(S_1, S_2)$ that simultaneously satisfies these two functions $6$ and $\rho$. Once the SRV pair is found, $D_p \alpha_1^2$ is computed and subtracted from $k_1$ to yield the bulk lifetime; that is, $k_1 - D_p \alpha_1^2 = 1/\tau_b$.

5.4 The Separation Algorithm

The crux of the separation of recombination parameters is the iterative routine which finds the pair of SRVs $(S_1, S_2)$ from $6$ and $\rho$, which are both non-linear functions of the SRVs. A number of different separation routines are possible, but it most logical to employ the knowledge gained in chapter 4 to construct an algorithm.

5.4.1 The reasoning used to construct the algorithm

The decay coefficients $k_i$ are the sum of the inverse bulk lifetime and the inverse surface lifetime, for example, $k_i = D_p \alpha_i^2 + 1/\tau_b$. The bulk lifetime is the same in every $k_i$, whereas the surface lifetime $D_p \alpha_i^2$ increases approximately as $i^2$. Therefore, the bulk lifetime term contributes far less to higher-order terms, meaning that the larger the index $i$ the more independent of bulk lifetime is that particular $k_i$.

Since the $\alpha_i$ increase monotonically with the average S value $\bar{S}$, it is correct to qualitatively think of them interchangeably. As $S$ increases, so does $\alpha_i$, so that upper limits on $\alpha_i$ prescribe upper limits on $\bar{S}$. In addition, since the $\alpha_i$ values increase with index $i$, a greater proportion of $k_2$ is the surface term $D_p \alpha_2^2$, since $\alpha_i$ for even nominal sample widths are very large for $i = 2$ and higher terms.

5.4.2 The iterative separation routine

To satisfy the functions $6$ and $\rho$, some process of guessing must be used to find $(S_1, S_2)$. Of the decay parameters $\{C_1, C_2, k_1, k_2\}$, $k_2$ most nearly isolates a recombination parameter directly. That is, since $D_p \alpha_2^2$ is likely to dominate $k_2$, $k_2 \approx D_p \alpha_2^2$, so that dividing $k_2$ by $D_p$ and taking its square root yields an upper bound on $\alpha_2$, that is, $\sqrt{k_2/D_p} \approx \alpha_2$. Per the above discussion, we know that $\alpha_2$ prescribes the greatest upper bound on $\bar{S}$ via the eigenvalue eqn. 4.4. This maximum $\bar{S}$, in turn, fixes the greatest upper bound on either $S$ (which is $2\bar{S}$), since $\Delta S \in [0, \bar{S}]$. Thus, by this calculation on $k_2$, definite bounds are set on the maximum value of either $S$. By this process, a search can be
performed for the actual S values by sequentially lowering the upper bounds that are obtained, in a monotonically decreasing fashion.

The above calculation yields the maximum $S$ and $\alpha_2$; therefore, considering these to be the actual values, they are inserted into a routine which searches through $\rho = C_2/C_1$ for the pair of actual $(S_1, S_2)$ that satisfies it. Once this pair is found, the value of $\alpha_1$ is calculated from $(S_1, S_2)$ using the eigenvalue eqn. 4.4, so an upper bound can be found for the bulk lifetime, $\tau_b = 1/(k_1 - D_p\alpha_1^2)$.

Now, $1/\tau_b$ (which is the least lower bound) is subtracted from $k$, to find a better estimate for $\alpha_2$, which begins the iterative loop anew. The above process is repeated, and at the end of the loop, the bulk lifetime obtained is compared with the bulk lifetime obtained from the previous loop to test for convergence. Because of the way in which the definite bounds are interdependent within the routine, this scheme should be eminently stable because no overshooting estimates can occur; the routine just iterates until it converges. Figure 5.1 below pictorially depicts the complete algorithm.

5.4.3 Flip-over strategy for consistency checks

Since the PCD theory presented provides for two independent surface recombination velocities, a simple verification of the recombination parameters (and the theory) is provided by taking a second PCD measurement with the sample inverted (flipped over). The inverted PCD data should appear different, yet be related in a quasi-conjugate fashion, and producing identical results for all of the recombination parameters. Alternatively, this flip-over strategy also provides another independent function of the decay parameters, $\rho_{inv} = (C_2/C_1)_{inv}$, which would allow for the diffusivity $D_p$ of the sample to be independently determined.

Consider now the expected values of $\delta_{inv}$ and $\rho_{inv}$. If the theory is correct in all of its assumptions, flipping the sample over to obtain a second PCD decay curve should ideally have as its sole result the exchange of $S_1$ and $S_2$ in all of the functions and parameters. Practically speaking, there might be measured changes induced in the flip-over caused by the asymmetric absorption of the excitation beam (which would change the injection level at the excited surface as compared with the dark surface) and any effect on the probe caused by differences in surface roughness. These, in addition to the validity of the basic assumptions of the theory, must have negligible effect for the following assertions about the flipped-over measurement results to hold true.
Fig. 5.1: Flow diagram for the separation algorithm.
Measure sample thickness and assume a value of diffusivity based on sample doping.

Make PCO measurements to obtain a decay curve.

Apply ESPRIT to the curve to obtain the decay coefficients, and then apply least squares to find the amplitudes.

(Begin the separation algorithm)
Estimate $\alpha_2$ and $S_{\text{max}}$ from $k_2$.

Using $\alpha_2$ and $S_{\text{max}}$, find $S_1$ and $S_2$ from the ratio $C_2/C_1$.

Using this $S_1$ and $S_2$, compute $\alpha_1$ and then estimate $r_0$ from $k_1$.

Test for convergence by comparing $r_0$ with previous $r_0$.

Convergence.
From the previously presented symmetry/asymmetry arguments for $\delta$ and $p$, the values of $\delta_{\text{inv}}$ and $p_{\text{inv}}$ can easily be found, both quantitatively and qualitatively. Since the $\alpha_i$ are symmetric functions of the SRVs, all of the $k_i$ obtained from the flipped-over measurement should be the same as those from the initial measurement. Therefore, $\delta_{\text{inv}} = k_2 - k$ should equal $\delta$. (For a visual verification of this, consider figures 4.4 and 4.8.) The value obtained for $\delta_{\text{inv}}$ for any value of $(S_1, S_2)$ is the mirror image across the main floor diagonal of the value obtained for $\delta$.

Conversely, because of the asymmetry of $p = C_2/C_1$, the value of $p_{\text{inv}}$ will be quite different from $p$, and should have opposite algebraic sign. This can be seen from figures 4.5 and 4.7 by again taking the mirror image point about their main floor diagonals.

As was mentioned above, the comparison of flipped-over results with the original results provides a simple test of the present theory and all of its assumptions. Alternatively, it can be viewed as a means by which to alter the measurement parameters in order to bring them into line with the theory for the purpose of assuring correct results. In addition, this flip-over verification costs nothing, and is contactless and non-destructive.

### 5.5 Chapter Summary

The complete method for deducing the recombination parameters from PCD data has been presented. The method has four aspects: measurement of sample thickness and diffusivity, a PCD measurement under proper conditions, extraction of the parameters of the PCD curve using ESPRIT, and separation of the recombination parameters from the PCD parameters using a convergent iterative routine. The iterative routine employs the properties of the PCD parameters to provide continually shrinking bounds on the parameters, so that it should be very stable.

In addition, the procedure for a self-consistency check on the theory and method was presented, through comparison of the measurement of the inverted sample with the original measurement. Because of the properties of the parameters in the theory, this flip-over method is a direct test of the validity of the assumptions, theory, and results, and is quite simple to perform.
This page intentionally left blank.
6. EXPERIMENTAL RESULTS AND ANALYSIS

6.1 Introduction

Employing the separation algorithm set forth in chapter 5, some experimental data from silicon samples will now be analyzed to discover whether the separation of bulk and surface recombination is possible in practice. It should be noted that the successful application of the present method does not depend upon the separation algorithm nor specifically the expressions comprising the theory, but on the validity of the theory for describing a µW-PCD measurement under the specified conditions; the method should be successful if the restrictions placed on the theory can be attained.

The requirements for validity of the theory are that the excess carriers are (always and everywhere) in a low-injection condition within the sample; that the surface recombination velocities, bulk lifetime, and carrier diffusivity remain constant throughout the measured photoconductivity decay curve. In addition, there must be no sensitivity of the detection system to carrier distribution or transport, and no other unaccounted-for detection effects.

The requirements placed on the apparatus are that sampling of the decay must take place at a rate sufficient to provide a density of data points for the accurate extraction of the two lowest-order decay coefficients and amplitudes. (As material quality and lifetimes increase, this latter condition becomes easier to satisfy.) It is also assumed that the thickness of the sample can be measured, that the diffusivity of the sample can be found through doping or resistivity measurements, and the absorption coefficient of the excitation source can be found or computed.

6.1: Data Analysis

Through the cooperation of Paul Basore of Sandia National Laboratories and Richard Ahrenkiel of the National Renewable Energy Laboratories, several sets of photoconductive decay data (microwave-detected and inductively-coupled, respectively) were provided. For all of the microwave-detected data, the microwave probe was 9.6 GHz
TE10 mode issuing from an open rectangular waveguide, and a GaAs laser diode exciter (904 nanometers, absorption coefficient = 294/cm) was used. The inductively coupled apparatus used a frequency of 400 MHz, and a Nd:YAG laser excitation source; this exciter was used at both 532 nanometers (green, absorption coefficient = 7000/cm) and 1064 nanometers (infrared, absorption coefficient = 11/cm), directed through an adjustable polarizer to reduce its intensity as needed.

Figure 6.1 below shows the appearance of measured data, obtained using microwave detection. The transient is negative because the slope of the reflectance versus conductivity is negative (i.e., to the left of the minimum of figure 2.3). To extract the parameters of this decay curve, the rapid initial transient was removed and the time axis shifted to the right such that the first data point on a par with the maximum is taken as the time origin.

![Figure 6.1](image)

Fig. 6.1: The appearance of a measured microwave-detected PCD decay curve.

Figure 6.2 displays the time-shifted and inverted data from figure 6.1, which is the result of a μW-PCD measurement on a 4-inch round, n-type Wacker float-zone sample. The data is the average of 2,048 trials, and is composed of 500 data points taken at 0.1 microsecond intervals. Using a measured thickness of W=380 micrometers and an assumed diffusivity of 10 cm²/sec, the algorithm produced a bulk lifetime of 0.54
milliseconds, and respective surface recombination velocities (SRVs) of 854 cm/sec at the (unpolished) illuminated surface and 75 cm/sec at the dark surface. The usual μW-PCD analysis of the data would have yielded an effective lifetime of 66.8 microseconds. By this, it can be seen that the SRVs, not the bulk lifetime, are the factors limiting the effective lifetime of the sample.

![Graph](image)

**Fig. 6.2**: Measured μW-PCD data; sample and sampling parameters as displayed.

Since the algorithm was successful for this sample, it is useful to consider the features of this curve further to gain some insight into its success. Figure 6.3 below shows a semilogarithmic plot of the same data that appears in figure 6.2 (and 6.1). The linear portion to the right of the data shows that it was sampled for a duration sufficient to ensure that the final, single-exponential mode was attained. During the course of this work, PCD decay curves were synthesized from the expressions and it was found that the data must include the lowest order mode in isolation as a necessary condition for the ESPRIT algorithm to function correctly (which requires that the sampling duration must continue until the final decay mode has been attained.) In practice, this implies that the initial excitation must be great enough (while yet causing only low-injection) so that the final decay mode appears before the "noise floor" of the measurement system is reached (although averaging a large number of trials may somewhat reduce the effects of the noise.)
This requirement may also limit the maximum SRVs for which this method is valid, since as SRVs increase so do the relative amplitudes of the higher order modes; that is, if the higher-order modes are "too large," they may dominate the decay curve making it **impossible** to find the lowest-order mode in isolation.

![Fig. 6.3: Semilog plot of the μW-PCD data from fig. 6.2.](image)

Moving to another data set, figure 6.4 below shows a different μW-PCD sample; the data meets the requirement of attaining final mode. Qualitatively, it can be said that either the surface recombination velocities (SRVs) are equal or very small (or both), since the entire decay curve is virtually a single exponential. The sample was n-type float zone Silicon with approximately 20 nanometers of thermal oxide passivation on its surfaces. It is not known whether both sides were polished. Since it is obvious that the decay rapidly settles into its final decay (the straight line portion on the plot), it is not necessary to use all of the data points in order to extract the decay parameters using ESPRIT. Using the first 200 data points in ESPRIT produced acceptable-looking decay coefficients of $k_1=1.1729\times10^3$, $k_2=5.1268\times10^3$, and $k_3=1.2862\times10^5$, as well as amplitudes of $C_1=0.86645$, $C_2=0.038622$, and $C_3=0.12092$. However, when these numbers where input to the solver, along with a minority hole diffusivity of 12.7, the algorithm showed that this diffusivity was an order of magnitude too large. This demonstrated that the
second-order mode values were invalid according to the theory. In consideration of this, the second-order mode values were discarded and replaced with the third-order mode values obtained (under the assumption that the second-order modes were due to spurious curvature of the PCD data.) Using these values, the algorithm produced a negative bulk lifetime value, indicating too much spacing between the decay coefficients $k_i$; therefore, the early features of the decay curve are not according to theory, causing the separation method to fail for this particular data set. This failure is clearly signaled by rejection of the diffusivity value as "out of range," or impossible values (e.g., negative bulk lifetime) for the recombination components, which are beneficial features of the theory presented in Chapter 4.

![Fig. 6.4: A measured μW-PCD decay with small surface recombination velocities.](image)

It is useful to consider the possible sources of the early, rapid decay of figure 6.4. The candidate factors that might have produced the early decay bump are: the non delta function excitation, variable surface recombination velocities, or momentary high-injection. (These samples are non-diffused and unprocessed; therefore position-dependent bulk lifetime is ruled out as a possible cause.) For relative comparison, figure 6.5 below shows the results of a measurement on the same sample, differing only in that it included
approximately 0.2 Suns of red-light bias. This light-biased curve lacks the early decay drop that appears in figure 6.4, so it can give clues as to the origin of that drop.

In figure 6.5, the overall injection level throughout the sample is increased because of the light bias, yet the plot shows no sign of an early drop. Both figures share the same exciter, so that the shape of the excitation pulse should be ruled out as the cause of the initial drop. The effective lifetime from figure 6.4 is about 850 µs, whereas from figure 6.5 (with light bias) the effective lifetime was computed as 2.4 ms, almost a threefold increase. Therefore, since the lifetime in figure 6.5 is greater, rather than less than in figure 6.4, high injection cannot be the cause of the early drop in figure 6.4 (which decays more rapidly than the remainder of the curve.) Therefore, a possible explanation for the early drop in figure 6.4 as well as the relative increase of effective lifetime in figure 6.5 is that the light-bias has saturated the surface states with minority carriers, reducing the surface recombination velocities at higher injection levels. Figure 6.5 is a single exponential, implying that the surface recombination velocities are identically zero (there are no modes with indices higher than 1 and the effective lifetime is the true bulk lifetime of the sample.)

![Fig. 6.5: μW-PCD curve with 0.2 Suns red-light bias.](image)
Considering another sample, figure 6.6 shows the results from an n-type sample, doped about $1 \times 10^{14}$, and which is 620 $\mu$m thick. This sample had the oxide completely stripped, and was measured in air. The exciter beam was the infrared line of the YAG laser, 1.054 $\mu$m. The figure shows a marked concave-down feature, indicating (as did figure 6.5) that the recombination rate is increasing as the injection level decreases. Accordingly, the separation analysis attempt produced unacceptable results. The concave-downwards shape is possible for some highly-absorbed exciter beams, but this should never occur at the end of the decay; for the mildly absorbed exciter used in this example, this shape can never occur. That it is occurring so strongly for this sample is most probably due to the fact that this sample had its oxide stripped before measurement, which drastically increases the number of available surface states, and hence the SRVs of the sample; the larger the SRVs, the greater the relative variations possible. The shape of the decay curve is an immediate indication that this sample violates of the assumptions of the theory.

![Inductively-detected PCD measurement curve](image)

**Fig. 6.6:** An inductively-detected PCD measurement curve; noise on the right of the figure is due to digitization error.

The concave-downwards results can be explained by an analysis performed by Ahrenkiel [56]. In that paper, a study of the injection-level dependence of Shockley-Read-Hall recombination described the variation of bulk lifetime with injection level due to saturation of traps. For large differences in minority and majority capture cross sections of
a single level, it was demonstrated that majority-carrier capture can be the limiting factor determining recombination rates at higher injection levels. Qualitatively, this is described as a trap saturation effect that causes bulk lifetime to decrease as injection level decreases. Samples in which this occur are outside the scope of the validity of the present technique, but can visually be identified by the concave-downwards shape.

6.3 Paired Measurements to Test for Self-Consistency of the Technique

Chapter 5 described a simple test that could be used to verify the validity of the present technique, using self-consistency between measurements on either side of a sample. Several sets of data were data were considered with this in mind. According to the theory, these two measurements would be consistent if the corresponding decay coefficients $k_i$ are identical in both measurements and that the amplitude ratio $C_2/C_1$ is some number that yields invariant SRVs for each of the sample sides. (A visual test that both values of $k_1$ are equal is that the final decay "tail" has the same slope on both sides of samples.)

Figure 6.7 depicts a family of pairs of microwave-detected PCD curves from a single sample. They are from a p-type Czochralski sample, 634 microns in thickness, 8 ohm-cm resistivity. Each pair of curves is a front-side/back-side pair, and the five pairs correspond to different intensities of the GaAs exciter beam. The higher curve of each pair is the measurement taken with the exciter illuminating the single polished side of the sample.
Fig. 6.7: Five pairs of front-back side \( \mu \text{W-PCD} \) measurement pairs. The laser drive currents, in descending order, are 40 mA, 35 mA, 30 mA, 25 mA, 20 mA. The upper curve of each pair had the incident beam on the polished side of the sample.

These curves were subjected to ESPRIT in order to obtain their decay parameters. It was expected that \( C_2 \) for each of the "back side" (higher) curves would be negative for this highly-absorbed beam, since the unpolished (and therefore higher recombination) surface was on the far side of the sample from the exciter. (This is the result that would occur if the SRVs were invariant whether excited or not.) ESPRIT did not obtain these expected results; however, this does not negate the validity of the theory, but rather the self-consistency test described in chapter 4.

The curves in figure 6.7 were analyzed to separate bulk lifetime and surface recombination velocities; the results are listed in table 6.1. Table 6.2 lists the effective lifetime results for the same measurement conditions upon the same sample. To display the goodness of fit of the ESPRIT results, decay curves were synthesized from the ESPRIT extracted parameters and plotted with the original data in figures 6.9 through 6.13.
Table 6.1
ESPRIT and separation results for the various curves in fig. 6.7; paired sets of results are in descending order, as in fig. 6.7. Curve fits calculated from decay parameters \((C_i, k_i)\) are shown in figs. 6.9 through 6.13.

<table>
<thead>
<tr>
<th>Laser current</th>
<th>UPPER CURVES</th>
<th>LOWER CURVES</th>
</tr>
</thead>
<tbody>
<tr>
<td>40 mA</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(\tau=88\ \mu s), (S_1=2480, S_2=582)</td>
<td>(C_1=1.303, k_1=1.520e4)</td>
<td>(C_1=1.117, k_1=1.902e4)</td>
</tr>
<tr>
<td>(C_2=0.4038, k_2=1.659e5)</td>
<td>(C_2=0.5654, k_2=1.955e5)</td>
<td></td>
</tr>
<tr>
<td>35 mA</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(\tau=55\ \mu s), (S_1=3588, S_2=944)</td>
<td>(C_1=0.6866, k_1=1.691e4)</td>
<td>(C_1=0.5676, k_1=1.969e4)</td>
</tr>
<tr>
<td>(C_2=0.2844, k_2=1.927e5)</td>
<td>(C_2=0.4451, k_2=1.910e5)</td>
<td></td>
</tr>
<tr>
<td>30 mA</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(\tau=59\ \mu s), (S_1=3542, S_2=909)</td>
<td>(C_1=0.4062, k_1=1.841e4)</td>
<td>(C_1=0.3437, k_1=2.219e4)</td>
</tr>
<tr>
<td>(C_2=0.1071, k_2=2.212e5)</td>
<td>(C_2=0.1628, k_2=2.343e5)</td>
<td></td>
</tr>
<tr>
<td>25 mA</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(\tau=44\ \mu s), (S_1=5292, S_2=1286)</td>
<td>(C_1=0.1406, k_1=2.142e4)</td>
<td>(C_1=0.1138, k_1=2.285e4)</td>
</tr>
<tr>
<td>(C_2=0.02798, k_2=2.695e5)</td>
<td>(C_2=0.05653, k_2=1.921e5)</td>
<td></td>
</tr>
<tr>
<td>20 mA</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(\tau=48\ \mu s, S_1=4490, S_2=1515)</td>
<td>(C_1=0.1138, k_1=2.285e4)</td>
<td>(C_1=0.1138, k_1=2.285e4)</td>
</tr>
<tr>
<td>(C_2=0.02798, k_2=2.695e5)</td>
<td>(C_2=0.05653, k_2=1.921e5)</td>
<td></td>
</tr>
</tbody>
</table>

Table 6.2
Measured effective lifetimes for conditions of fig. 6.7, measured at Sandia National Laboratories. Values were measured between 50 and 100 \(\mu s\), rather than between 0 and 50 \(\mu s\) as in fig 6.7.

<table>
<thead>
<tr>
<th>Laser current</th>
<th>UPPER CURVES</th>
<th>LOWER CURVES</th>
</tr>
</thead>
<tbody>
<tr>
<td>40 mA</td>
<td>70.62 (\mu s)</td>
<td>68.6 (\mu s)</td>
</tr>
<tr>
<td>35 mA</td>
<td>67.92 (\mu s)</td>
<td>65.21 (\mu s)</td>
</tr>
<tr>
<td>30 mA</td>
<td>65.72 (\mu s)</td>
<td>63.51 (\mu s)</td>
</tr>
<tr>
<td>25 mA</td>
<td>62.74 (\mu s)</td>
<td>60.48 (\mu s)</td>
</tr>
<tr>
<td>20 mA</td>
<td>55.58 (\mu s)</td>
<td>53.99 (\mu s)</td>
</tr>
</tbody>
</table>
Each of the curves produced reasonable decay parameters in ESPRIT, and yielded valid numbers from the separation technique. Although there are no absolute trends across the series of curves, the surface recombination velocity at the excited surfaces is always greatest, often by a factor of four, regardless of their polished or unpolished condition. The surface recombination velocity at the excited surface ranges from 2480 to 9158, while the unexcited SRVs are in the range from 497 to 1515. The curves for which the best fits were obtained (figures 6.10 and 6.11) produced results that are in excellent agreement with each other. Excluding the noisy data pair (25 mA laser current), each of the pairs produced bulk lifetimes that agreed within a factor of two.

The Sandia results in table 6.2 do not perfectly correspond to the (effective) lifetimes that could be obtained from the data of figure 6.7, since the former were measured on a longer time scale. However, they are provided for comparison purposes, and demonstrate that the lifetime values obtained are similar. The Sandia results show that shorter effective lifetimes were obtained at lower intensity levels; if bulk lifetime was constant, the surface recombination velocities were greatest at lowest illumination levels.

The reason that the excited SRVs were always greatest will now be considered. The ratio of the intensity of the exciter between the uppermost and lowermost pair of curves is about 2:1. If high-injection near the excited surface were the cause of the rapid, early decay, this condition should appear as more rapid early drops in the higher amplitude curves. However, this is probably not the case, since the set of all front-side decay curves (the lower curve of each pair) is approximately parallel, as is the set of all back-side decay curves (the higher curve of each pair). Because of the relative constancy of the results and the parallelism of the curves, it is doubtful that high injection is occurring to any extent in the measurement samples at any of the levels. Therefore, the following explanation is offered.

Fixed oxide charge is usually found to be positive; for this p-type sample, this means that there is a surface accumulation of minority electrons at the surface, and some downwards band-bending when the sample is in equilibrium. The bent bands mean that the Fermi level at the surface is near the intrinsic level (for this relatively low-doped sample); the mid-gap states in this region are the most effective recombination centers. In addition, for donor-like states, electron capture coefficients are much greater than for majority holes. At the instant of excitation, the region near the surface of the sample is flooded with electron-hole pairs; the surface field due to oxide charge would draw minority electrons to it, which flattens the bands near the surfaces. This flattening of the bands simultaneously bares the very efficient mid-gap interface states for electron capture, as well as allowing
majority holes to relax towards the surface. The confluence of these transient effects acts to briefly increase the recombination rate at the excited surface until band-bending again regains its former state (see figure 6.8). (That the separation produces an excited SRV is not necessarily bad; it is the illuminated SRV that is of importance during solar cell operation.)

Fig. 6.8: (a) The upper diagram depicts the equilibrium condition of a lightly doped p-type sample with positive fixed oxide charge. (b) The lower figure depicts the condition of the same material, just after excitation has flattened the surface bands. (Free carriers in bands not shown.)
Fig. 6.9: The curves of highest amplitude (40 mA laser drive current) from fig. 6.7, and their fit curves. The fitted curves extend past the end of the measured curves for identification purposes.
Fig. 6.10: The curves of second highest amplitude (35 mA laser drive current) from fig. 6.7, and their fit curves. The fitted curves extend past the end of the measured curves for identification purposes.
Fig. 6.11: The curves of third highest amplitude (30 mA laser drive current) from fig. 6.7, and their fit curves. The fitted curves extend past the end of the measured curves for identification purposes.
Fig. 6.12: The curves of fourth highest amplitude (25 mA laser drive current) from fig. 6.7, and their fit curves. The fitted curves extend past the end of the measured curves for identification purposes.
Fig. 6.13: The curves of lowest amplitude (20 mA laser drive current) from fig. 6.7, and their fit curves. The fitted curves extend past the end of the measured curves for identification purposes.
6.4 Conclusions

Measured PCD data from several samples was successfully analyzed using ESPRIT and the separation technique. Some pathologies in data can often be rejected by testing for proper differences in decay coefficients $k_i$ or visual recognition of disallowed shapes and features in curves.

The flip-over test for self-consistency of the results revealed that the excited SRVs are always larger; therefore, it is not possible to test for self-consistency in the sense described in Chapter 5 (under the expectation that an SRV will not change when illuminated). The test did show a positive correlation between SRV and unpolished condition of the surface. The bulk lifetime results from each side were in agreement within a factor of two.
7. CONCLUSIONS AND SUGGESTIONS FOR FUTURE WORK

7.1 Summary

A data analysis method has been presented for finding values for the bulk lifetime and both surface recombination velocities of a sample, using only one set of measurement results. The method is nondestructive and requires only a suitable computer, a thickness measurement, a minority-carrier diffusivity value, and the absorption coefficient of the excitation source in addition to a standard contactless (either microwave or inductively-coupled) Photoconductive Decay apparatus. This method has the novelty that it uses computations, rather than the physical manipulation of a measurement parameter, to accomplish the separation. This computational separation is made possible by a depth-insensitive excess carrier probe, which allows the minority carrier distributions to be integrated across the measurement sample, leaving the total photoconductive decay signal as the infinite sum of decaying exponentials whose decay coefficients are on different time scales. The extraction of the amplitudes and decay coefficients of the lowest two or three exponentials from measurement data allows them to be combined such that the surface recombination velocities and the bulk lifetime sample can be uniquely extracted by self-consistent calculations. The theory is quite extensive and has many useful features; however, the success of the technique depends entirely on the ability of the rather idealized theory to adequately explain the carrier decay kinetics.

The present method should prove to be quite robust, for several reasons. First, there is a redundant amount of information available through the extracted parameters, which allows for consistency checks. Also, spurious decay harmonics that may occur in the data due to non-linearities in the reflectance characteristic can often be rejected on the basis of the theory of this method, which prescribes limited ranges within which the decay coefficient differences must fall.
7.2 Conclusions and Suggestions for Further Study

The theory and interpretation of results from the widely-used Photoconductive Decay technique has been extended; it now includes two separate surface recombination velocities and provides explanations for the early features of decay curves. The computational separation method appears to be valid for a restricted range of sample parameters rather than for general application; however, this range of validity appears to appropriate to its intended use (pre-screening of solar cell starting materials).

In the previous chapter, experimentally obtained data was analyzed using the computation separation method to test its validity. The method produced acceptable results for most samples; other samples contained pathologies that could be identified visually or by the decay coefficient difference test.

Since the computational separation technique is nondestructive, many other methods can be used to post-verify its results, including techniques that passivate the surfaces, or crude methods like sandblasting, which drastically increases surface recombination. Other lifetime measurement techniques could also be used as cross-checks of the method.

It is suggested that the best manner in which to determine whether the present method is workable in practice would be to endeavor from the experimental side to determine how to simultaneously ensure all of the proper measurement conditions (e.g., low-injection everywhere, no lateral diffusion due to small spot-size). In addition, it is possible that ESPRIT is not necessarily the best algorithm for extracting the decay parameters from measurement data; perhaps a better technique applies in this situation. More work could be done to determine the proper sampling rates and durations needed for beat parameter extraction.

The single phenomenon that appears to be the greatest threat to the success of the technique is the possibility that surface recombination may vary with injection level. However, there may be some technique by which this variation may be nullified, such as adding light bias. Alternatively, perhaps the variation of surface recombination can be studied through the combined use of computer simulations and PCD measurements on very thick samples such that single surfaces are isolated; the expressions [23] for single-surface consideration have already been worked out.

In a peripheral issue, those studying spatial lifetime mapping using microwave-detected PCD may make use of the reflectance theory in chapter 3, especially eqn. 3.1, to determine if second-order effects due to small-spot size are confusing the obtained results.
REFERENCES


This page intentionally left blank.
Appendix A: Derivation of the Excess Minority Carrier Distribution Expression

This derivation assumes the following:

**Low-level** injection conditions prevail;

**One** Cartesian spatial dimension, $x$;

Two distinct values of surface recombination velocity, $S_1$ and $S_2$, which remain constant;

A single diffusion coefficient, $D_p$, which remains constant;

A homogenous bulk lifetime $\tau_b$, which remains constant.

### A.1 Minority carrier diffusion equation

The starting point is the minority carrier diffusion equation; assuming that holes $\Delta p(x,t)$ are the minority carriers, it is

$$ \frac{\partial \Delta p}{\partial t} = D_p \frac{\partial^2 \Delta p}{\partial x^2} - \frac{\Delta p}{\tau_b} $$

where

$$ \Delta p = \Delta p(x,t). $$

### A.2 Validity of solving heat equation

It is now shown that the related, yet simpler "heat equation" can be solved instead of the minority carrier diffusion equation by pre-assuming a form for our solution. Let $\Delta p(x,t)$ be the hypothetical solution to the heat equation, where the heat equation is

$$ \frac{\partial \Delta p}{\partial t} = D_p \frac{\partial^2 \Delta p}{\partial x^2}. $$

Now, assume that

$$ \Delta p = \Delta p \exp(t/\tau_b) $$

and substitute this into the heat equation.
\[
\frac{\partial \Delta p}{\partial t} = D_p \frac{\partial^2 \Delta p}{\partial x^2}
\]
is equivalent to
\[
\frac{\partial[\Delta p \exp(t/\tau_b)]}{\partial t} = D_p \frac{\partial^2[\Delta p \exp(t/\tau_b)]}{\partial x^2},
\]
which, when computed, is
\[
\exp(t/\tau_b) \frac{\Delta p}{\tau_b} + \exp(t/\tau_b) \frac{\partial \Delta p}{\partial t} = \exp(t/\tau_b) D_p \frac{\partial^2 \Delta p}{\partial x^2}.
\]
Canceling and rearranging gives
\[
\frac{\partial \Delta p}{\partial t} = D_p \frac{\partial^2 \Delta p}{\partial x^2} - \frac{\Delta p}{\tau_b},
\]
which is the minority carrier diffusion equation. Therefore, it is always valid to solve the simpler heat equation, multiplying the final result \( \Delta p \) by \( \exp(-t/\tau_b) \) in order to obtain the solution to the associated minority carrier diffusion equation.

### A.3 Series solution

By page 114 of Carslaw and Jeager [28], the boundary-value heat equation
\[
\frac{\partial \Delta p}{\partial t} = D_p \frac{\partial^2 \Delta p}{\partial x^2}
\]
has an infinite series solution composed of eigenfunctions of the form
\[
\Delta p_i = \exp(-D_p \alpha_i^2 t)[A_i \cos(\alpha_i x) + B_i \sin(\alpha_i x)],
\]
where the \( \alpha_i \) are the eigenvalues of the equation.

(Note: The correspondences between the notation in Carslaw and Jeager and the notation in this appendix are the following: \( v \to \), \( h \to \), \( K \to D_p \), and \( 1 \to W \). Notice that the values of \( 'h' \) are set equal, not independent as we have them.)

The boundary conditions are:

- at \( x = 0 \),
  \[
  \frac{\partial \Delta p}{\partial x} = \frac{S_1}{D_p} \Delta p
  \]
- and at \( x = W \),
  \[
  \frac{\partial \Delta p}{\partial x} = -\frac{S_1}{D_p} \Delta p
  \]

Now, applying the first boundary conditions to an eigenfunction at \( x=0 \) yields
\[
\frac{\partial \Delta p}{\partial x} = \frac{S_i}{D_p} \Delta p
\]

is

\[
[-\alpha_i, A_i \sin(\alpha_i, 0) + \alpha_i, B_i \cos(\alpha_i, 0)] = \frac{S_i}{D_p} [A_i \cos(\alpha_i, 0) + B_i \sin(\alpha_i, 0)]
\]

which is

\[
\alpha_i B_i = \frac{S_i}{D_p} A_i,
\]

or

\[
B_i = \frac{S_i}{\alpha_i D_p} A_i.
\]

This eliminates the constant \(B_i\) in the general eigenfunction form, yielding as the general solution for each \(i\)

\[
\Delta p_i = A_i \exp(-D_p \alpha_i^2 t) [\cos(\alpha_i x) + \frac{S_i}{\alpha_i D_p} \sin(\alpha_i x)]
\]

At the other boundary \((x=W)\),

\[
\frac{\partial \Delta p}{\partial x} = -\frac{S_i}{D_p} \Delta p
\]

is

\[
A[-\alpha_i \sin(\alpha_i W) + \alpha_i \frac{S_i}{\alpha_i D_p} \cos(\alpha_i W)] = -\frac{S_i}{D_p} A[\cos(\alpha_i W) + \frac{\varepsilon_i}{\alpha_i D_p} \sin(\alpha_i W)]
\]

or

\[
[-\alpha_i \sin(\alpha_i W) + \frac{S_i}{\alpha_i D_p} \cos(\alpha_i W)] = -\frac{S_i}{D_p} [\cos(\alpha_i W) + \frac{\varepsilon_i}{\alpha_i D_p} \sin(\alpha_i W)]
\]

Rearranging this gives

\[
\left( \frac{S_i S_2}{\alpha_i D_p^2} - \alpha_i \right) \sin(\alpha_i W) = -\frac{S_i}{D_p} - \frac{S_i}{\alpha_i D_p} \cos(\alpha_i W)
\]

or

\[
\tan(\alpha_i W) = \frac{-S_i - S_i}{D_p \left( \frac{S_i S_2}{\alpha_i D_p^2} - \alpha_i \right)}
\]

which is
This final equation is the transcendental eigenvalue equation for finding \( \alpha_i \) for each \( i \).

The initial condition (at \( t = 0 \)), assuming the excitation beam's time-dependence is a delta-function, is:

\[
\sum_{i=1}^{\infty} A_i \exp(-D_p \alpha_i^2 t) [\cos(\alpha_i x) + \frac{S_i}{\alpha_i D_p} \sin(\alpha_i x)] = \gamma F \exp(-\gamma x).
\]

For brevity, denote

\[
X_i = [\cos(\alpha_i x) + \frac{S_i}{\alpha_i D_p} \sin(\alpha_i x)].
\]

Therefore, again,

\[
\sum_{i=1}^{\infty} A_i X_i = \gamma F \exp(-\gamma x).
\]

This equation gives the values of \( A_i \) for \( i \).

Using the orthogonality property of the \( X_i \) in order to isolate the \( A_i \), multiply both sides by \( \sum_{i=1}^{\infty} X_i \) and integrate across the domain:

\[
\int_0^W dx \left\{ \sum_{i=1}^{\infty} A_i \sum_{i=1}^{\infty} X_i \right\} = \int_0^W dx \left\{ \sum_{i=1}^{\infty} X_i \gamma F \exp(-\gamma x) \right\}.
\]

Orthogonality and the interchange of the limiting operations simplifies this expression to:

\[
\sum_{i=1}^{\infty} A_i \int_0^W dx X_i = \gamma F \sum_{i=1}^{\infty} \int_0^W dx \left\{ \exp(-\gamma x)[\cos(\alpha_i x) + \frac{S_i}{\alpha_i D_p} \sin(\alpha_i x)] \right\}
\]

where the solution for each \( i \) is independent. Therefore, for each \( i \),

\[
A_i = \frac{\gamma F \int_0^W dx \exp(-\gamma x)[\cos(\alpha_i x) + \frac{S_i}{\alpha_i D_p} \sin(\alpha_i x)]}{\int_0^W dx X_i^2}
\]

There are two integrals to solve. To avoid confusion, let the above equation be denoted
Let $N_i$, the normalization factor for $A_i$ and which is independent of the forcing function, be solved for first. Following Carslaw and Jeager [28], pp. 116-118,

$$N_i = \int_0^W dx X_i^2,$$

but by the form of the $X_i$,

$$\frac{d^2 X_i}{dx^2} = -\alpha_i^2 X_i,$$

so that

$$\int_0^W dx X_i \frac{d^2 X_i}{dx^2} = -\alpha_i^2 \int_0^W dx X_i^2.$$

Now, solving the left side, integrating by parts,

$$\int_0^W dx X_i \frac{d^2 X_i}{dx^2} = \left[ X_i \frac{dX_i}{dx} \right]_{x=0}^{x=W} - \int_0^W dx \left( \frac{dX_i}{dx} \right)^2.$$

The integral on the far right-hand side must be evaluated. First, adding

$$\left( \frac{dX_i}{dx} \right)^2 = \alpha_i^2 \sin^2(\alpha_i x) + \left( \frac{S_i}{D_p} \right)^2 \cos^2(\alpha_i x) - \frac{2\alpha_i S_i}{D_p} \sin(\alpha_i x) \cos(\alpha_i x)$$

to

$$\alpha_i^2 X_i^2 = \alpha_i^2 \cos^2(\alpha_i x) + \left( \frac{S_i}{D_p} \right)^2 \sin^2(\alpha_i x) + \frac{2\alpha_i S_i}{D_p} \sin(\alpha_i x) \cos(\alpha_i x)$$

gives the result that

$$\left( \frac{dX_i}{dx} \right)^2 + \alpha_i^2 X_i^2 = \alpha_i^2 + \left( \frac{S_i}{D_p} \right)^2$$

Therefore,

$$\int_0^W dx \left( \frac{dX_i}{dx} \right)^2 = -\alpha_i^2 \int_0^W dx X_i^2 + \left( \alpha_i^2 + \left( \frac{S_i}{D_p} \right)^2 \right) W.$$
\[ X_j^2(x) = \cos^2(\alpha_j x) + \left( \frac{S_j}{\alpha_j D_p} \right)^2 \sin^2(\alpha_j x) + \frac{2S_j}{\alpha_j D_p} \sin(\alpha_j x) \cos(\alpha_j x), \]

so that \[ X_j^2(0) = 1. \]

Also, from above, recall that

\[ \left( \frac{dX_j}{dx} \right)^2 + \alpha_j^2 X_j^2 = \alpha_j^2 + \left( \frac{S_j}{D_p} \right)^2 \]

Using the boundary condition on the left-most term, then solving for \( X_j^2 \) gives

\[ X_j^2(W) = \frac{\alpha_j^2 + \left( \frac{S_j}{D_p} \right)^2}{\alpha_j^2 + \left( \frac{S_j}{D_p} \right)^2}, \]

Thus, the surface term is

\[ \left[ X_j \frac{dX_j}{dx} \right]_{x=0}^{x=W} = -\frac{S_j}{D_p} \left( \frac{\alpha_j^2 + \left( \frac{S_j}{D_p} \right)^2}{\alpha_j^2 + \left( \frac{S_j}{D_p} \right)^2} \right) - \frac{S_j}{D_p}. \]

The total result for

\[ \int_0^W dx X_j \frac{d^2X_j}{dx^2} = \left[ X_j \frac{dX_j}{dx} \right]_{x=0}^{x=W} - \int_0^W \frac{dX_j}{dx} \frac{dX_j}{dx} \]

is thus

\[ -\frac{S_j}{D_p} \left( \frac{\alpha_j^2 + \left( \frac{S_j}{D_p} \right)^2}{\alpha_j^2 + \left( \frac{S_j}{D_p} \right)^2} \right) - S_j \frac{\alpha_j^2 + \left( \frac{S_j}{D_p} \right)^2}{\alpha_j^2 + \left( \frac{S_j}{D_p} \right)^2} \int_0^W dx X_j^2 - \left( \frac{S_j}{D_p} \right)^2 \right] W = -\alpha_j^2 \int_0^W dx X_j^2. \]

Now the original problem was to find the solution to

\[ N = \int_0^W dx X_j^2. \]

From above, we have

\[ -\frac{S_j}{D_p} \left( \frac{\alpha_j^2 + \left( \frac{S_j}{D_p} \right)^2}{\alpha_j^2 + \left( \frac{S_j}{D_p} \right)^2} \right) - S_j \frac{\alpha_j^2 + \left( \frac{S_j}{D_p} \right)^2}{\alpha_j^2 + \left( \frac{S_j}{D_p} \right)^2} \int_0^W dx X_j^2 - \left( \frac{S_j}{D_p} \right)^2 \right] W = -2\alpha_j^2 \int_0^W dx X_j^2. \]

so that
This can be checked by letting $S_1 = S_2 \equiv S$ and seeing that it reduces to the form found in Carslaw and Jeager [28], near the bottom of page 117.

Next, find the solution of

$$I_i = \int_0^w \! dx \exp(-\gamma x) \left[ \cos(\alpha_i x) + \frac{S_i}{\alpha_i D_p} \sin(\alpha_i x) \right].$$

Each term is a standard integral found in tables, for instance [37],

$$I_i = \frac{\exp(-\gamma x)}{\gamma^2 + \alpha_i^2} \left\{ (-\gamma - \frac{S_i}{D_p}) \cos(\alpha_i x) + (\alpha_i - \gamma \frac{S_i}{\alpha_i D_p}) \sin(\alpha_i x) \right\}_{x=0}^w \quad \text{which is}$$

$$I_i = \frac{1}{\gamma^2 + \alpha_i^2} \left\{ (\gamma + \frac{S_i}{D_p}) (1 - e^{-\gamma W}) \cos(\alpha_i W) + (\alpha_i - \gamma \frac{S_i}{\alpha_i D_p}) \sin(\alpha_i W) \right\}.$$

Combining the previous results, the solution for each $A_i$ is

$$A_i = \frac{\gamma F}{\gamma^2 + \alpha_i^2} \left\{ (\gamma + \frac{S_i}{D_p})(1 - e^{-\gamma W}) \cos(\alpha_i W) + (\alpha_i - \gamma \frac{S_i}{\alpha_i D_p}) \sin(\alpha_i W) \right\}$$

$$+ \frac{1}{2\alpha_i^2} \left\{ \frac{S_i}{D_p} \left( \frac{A_i^2 + \left( \frac{S_i}{D_p} \right)^2}{\alpha_i^2 + \left( \frac{S_i}{D_p} \right)^2} \right)^2 + \frac{S_i}{D_p} + \left\{ \alpha_i^2 + \left( \frac{S_i}{D_p} \right)^2 \right\} \right\} W.$$

To summarize this section, the solution to the heat equation is therefore

$$\overline{\Delta p} = \sum_{i=1}^{\infty} A_i \exp(-D_p \alpha_i^2 t) \left[ \cos(\alpha_i x) + \frac{S_i}{\alpha_i D_p} \sin(\alpha_i x) \right],$$

and the solution to the associated minority carrier diffusion equation is

$$\Delta p = \sum_{i=1}^{\infty} A_i \exp(-D_p \alpha_i^2 t) \left[ \cos(\alpha_i x) + \frac{S_i}{\alpha_i D_p} \sin(\alpha_i x) \right].$$
This page intentionally left blank.
Appendix B: Description Of The ESPRIT Technique

B.1 The ESPRIT method

The ESPRIT algorithm (Estimation of Signal Parameters by Rotational Invariance Techniques) is a method for extracting signals embedded in data [39]. The problem is formulated so as to find the generalized eigenvalues from two data sets differing only by a time (or spatial) shift. The method can be carried out in a number of ways; the algorithm explained below was chosen for its computational speed.

B.2 The basic form of the signal

Assume a time signal of the form \( x(t) = \sum_{i=1}^{p} C_i e^{-k_i t} \). In discrete-time (sampled) form, this is \( x_n = \sum_{i=1}^{p} C_i e^{-k_i n \Delta t} \), where \( n \) is the integer index of the data point in the time series. For simplicity of notation in the following discussion, rewrite this as \( x_n = \sum_{i=1}^{p} C_i r_i^* \) where \( r_i^* = e^{-k_i n \Delta t} \).

B.3 The mathematics of ESPRIT

Assume that the time series can be placed in a matrix in the following manner:

\[
X = \begin{bmatrix}
x_0 & x_1 & x_2 \\
x_1 & x_2 & x_3 \\
\vdots & \vdots & \vdots \\
x_{L-1} & x_L & x_{L+1}
\end{bmatrix}
\]

(To simplify the explanation, the examples will demonstrate the method used to find \( \mathbf{3} \) decay coefficients; hence, the \( \mathbf{3} \) columns of matrices \( X \) and \( Y \). Any number of decay coefficients can be sought.) \( L \) is the dimension of the sliding data window; the window is \( L \) points out of the total \( N \) data points. Similarly, a matrix \( Y \) can be defined, of the form
Now, $X$ can be written as

$$X = FC = \begin{bmatrix} 1 & 1 & 1 \\ r_1 & r_2 & r_3 \\ r_1^2 & r_2^2 & r_3^2 \\ \vdots & \vdots & \vdots \\ r_1^{L-1} & r_2^{L-1} & r_3^{L-1} \end{bmatrix} \begin{bmatrix} C_1 & r_1C_1 & r_1^2C_1 \\ C_2 & r_2C_2 & r_2^2C_2 \\ C_3 & r_3C_3 & r_3^2C_3 \end{bmatrix}.$$  

Similarly, $Y$ can be written as

$$Y = FC' = \begin{bmatrix} 1 & 1 & 1 \\ r_1 & r_2 & r_3 \\ r_1^2 & r_2^2 & r_3^2 \\ \vdots & \vdots & \vdots \\ r_1^{L-1} & r_2^{L-1} & r_3^{L-1} \end{bmatrix} \begin{bmatrix} r_1C_1 & r_1^2C_1 & r_1^3C_1 \\ r_2C_2 & r_2^2C_2 & r_2^3C_2 \\ r_3C_3 & r_3^2C_3 & r_3^3C_3 \end{bmatrix}.$$  

But,

$$C' = \Phi C = \begin{bmatrix} r_1 & 0 & 0 \\ 0 & r_2 & 0 \\ 0 & 0 & r_3 \end{bmatrix} \begin{bmatrix} C_1 & r_1C_1 & r_1^2C_1 \\ C_2 & r_2C_2 & r_2^2C_2 \\ C_3 & r_3C_3 & r_3^2C_3 \end{bmatrix},$$

so that $Y = F\Phi C$.

Now, the values on the diagonal of the matrix $\Phi$ are the eigenvalues $r_i$ sought. (That is, knowing the $r_i$, the decay coefficients $k_i$ are computed by the formula $k_i = -\ln(r_i)/\Delta r$.) One way to do this is to use singular value decomposition to find a basis for the column space of $X$ and $Y$, from which $X$ and $Y$ can be diagonalized. That is, perform

$$X = USV^T$$

where $S$ is of the form
\[
S = \begin{bmatrix}
\sigma_1 & 0 & 0 & 0 \\
0 & \sigma_2 & 0 & 0 \\
0 & 0 & \sigma_3 & 0 \\
0 & 0 & 0 & \sigma_4 \\
\vdots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & 0
\end{bmatrix}
\]

The \( \sigma_i \) are the singular values of \( X \); in columns of \( S \) where there are nonzero \( \sigma_i \), the corresponding columns of \( U \) contain orthonormal basis vectors for the column space of \( X \), and the corresponding columns of \( V \) contain orthonormal basis vectors for the row space of \( X \). In this case, 3 eigenvalues are sought, so the matrices \( U \) and \( V \) of 3 columns each are formed, which reduce \( X \) and \( Y \) to \((3 \times 3)\), giving

\[
X_1 = U_1^T XV_1 = U_1^T FCV_1,
\]

and

\[
Y_1 = U_1^T YV_1 = U_1^T F\Phi CV_1.
\]

Then,

\[
Y_1 - \lambda X_1 = U_1^T F(\Phi - \lambda I)CV_1,
\]

so that

\[
X_1^{-1}(Y_1 - \lambda X_1) = (X_1^{-1}Y_1 - \lambda I)
\]

where

\[
X_1^{-1}Y_1 = (U_1^T FCV_1)^{-1}U_1^T F\Phi CV_1 = (CV_1)^{-1}\Phi(CV_1).
\]

Therefore, finding the eigenvalues of \( X_1^{-1}Y \) yield the eigenvalues \( \lambda_i \) that we desire. From the \( \lambda_i \), the decay coefficients are \( k_i = \frac{-\ln(\lambda_i)}{\Delta t} \).

**B.4 Finding the amplitudes**

Once the \( \lambda_i \) are known, it is a matter of using least squares to find the amplitudes \( C_i \), \( C \approx r^\text{data} \), which is the right-division solution to the method.

\[
\hat{x} = \begin{bmatrix} x_0 \\ x_1 \\ \vdots \\ x_{N-1} \end{bmatrix} = F\hat{C} = \begin{bmatrix} 1 & 1 & 1 \\ r_1 & r_2 & r_3 \\ \vdots & \vdots & \vdots \\ r_1^{N-1} & r_2^{N-1} & r_3^{N-1} \end{bmatrix} \begin{bmatrix} C_1 \\ C_2 \\ \vdots \\ C_3 \end{bmatrix}
\]
B.5 A MATLAB script for realizing ESPRIT

Below is the Matlab "m.file" which performs the ESPRIT algorithm on PCD data. (Matlab is a commercial software package from "The Mathworks" Natick, Massachusetts, USA, phone (508) 653-1415.)

To use the script file below on a Unix-based system, enter the text below in a standard text file whose name ends in ".m" (for example, "esprit.m"). Start Matlab, then enter "esprit" (the file name that you chose, but without the ".m") and a carriage return; this will execute the file below. You will be prompted for the name of the file in which the data resides.

The data file must be in two column format, with the "time" axis in the first column and the "values" axis in the second column. The "time" axis is not used except to calculate the time step $\Delta t$ between adjacent data points.

Some important notes:

1) The script and data files must reside in the current directory in which Matlab is started.
2) The variable "L" must be chosen greater than "p", and $L < (N/\text{skip} \cdot p)$ for the algorithm to work properly. Typical values used have been: $N = 500$, $\text{skip} = 9$, $p = 2$ or $3$, $L$ in the range [40-100].

```matlab
% THIS FILE EXECUTES THE ESPRIT METHOD ON TWO-COLUMN DATA
format short e;
clear data N temp temp2 time K L p
clear x y r_hat C u s v u1 v1 r k

% PROMPT FOR THE INPUT FILE NAME
filename = input('Enter the data file name:', 's');
eval(['load ' filename]);
% READ THE TWO-COLUMN DATA INTO "DATA"
data = eval(filename);
% SEPARATE THE COLUMNS OF DATA
time = data(:,1);
data = data(:,2);
eval(['clear ' filename]);
```
%MAKE THE DATA POSITIVE, IF NOT ALREADY
if data(1,1) < 0.0
    data = -data;
end.

% PRINT THE NUMBER OF DATA POINTS
N := size(data);
N := N(1,1)

% PROMPT AND READ IN THE CALCULATION PARAMETERS
% THE FOLLOWING LINE ALLOWS ONE TO DECIMATE THE DATA
skip = input('Stepsize between data points? ');
% L IS THE NUMBER OF DATA POINTS TO USE
L = input('Use how many data points L (L+p)<(N/step)? ');
% p IS THE NUMBER OF EIGENVALUES TO FIND
p = input('Seek how many eigenvalues p (p must be less than L) ? ');

% DECIMATE THE DATA IF skip > 1
m=0;
for n=1:skip:N
    m = m+1;
    temp(m,1)=data(n,1);
    temp2(m,1)=time(n,1);
end
data=temp;
time=temp2;
N := size(data);
N := N(1,1)
K=N-L;

% LOAD THE X AND Y MATRICES
for n=1:K
    for m=1:L
        x(m,n)=data(n+m-1);
        y(m,n)=data(n+m);
end
end

% COMPUTE THE DECAY COEFFICIENTS
[u,s,v]=svd(x);

% FORM THE TRUNCATED BASIS MATRICES
u1=u(:,1:p);
v1=v(:,1:p);

% FIND THE EIGENVALUES
r=eig(inv(u1'*x*v1)*(u1'*y*v1));

% CALCULATE THE TIME-STEP
delT = time(2,1) - time(1,1);

% CONVERT THE EIGENVALUES INTO DECAY COEFFICIENTS
k=-log(r)/delT;

% NOW COMPUTE THE TERM AMPLITUDES;
% COMPUTE THE R MATRIX
for n=1:p
    for m=1:N
        r_hat(m,n) = r(n)^m-1;
    end
end

% (COMPUTE THE TERM AMPLITUDES
C=r_hat\data;

% PRINT THE RESULTS
C
k

% STORE THE RESULTS IN AN EXTERNAL FILE
outfile = ['R' filename int2str(L)]
fid = fopen(outfile,'w');
fprintf(fid,'%f\n',k);
fprintf(fid,'%f\n',C);
fprintf(fid,'\nabove are the MODE values\n');
fprintf(fid,'above are the COEFFICIENT values\n');
fprintf(fid,'results for DATASET %s\n
', filename);
fprintf(fid,'number of POINTS used = %d of %d\n', L, N);
fprintf(fid,'number of MODES SOUGHT= %d\n', p);
This page intentionally left blank.
Appendix C: Computer Code For Separation Of The Recombination Parameters From PCD Data

The following C code is one implementation of the separation algorithm. Much more error checking could be included in the code, but this initial version concentrated on functionality rather than completeness. Many thanks to Sho Kuwamoto for many of the root-finding routines.

#include <stdio.h>
#include <math.h>

#define STEPS 10
const int StepNum=500;
double gjącym;
double RatioTolerance;
double rat(double x);
double a1, a2, a3, b1, b2, U2-1, G, U, ratio21, W, b_sum, F;

const double PI =3.1415926535897932384626433;
const double PIPI=9.8696044010893586188344909;
const double minU3_1 = 39.4784176;
const double maxU3_1 = 78.95683521;
const double minU2_1 = 9.869604401;
const double maxU2_1 = 29.6088132;
double Bmin, Bmax, Bavg;

int Choose(double ratio21);
void SetBmax();
double equal(double);
double diff(void);
double ratio(double b0);

typedef double (*dFunc)(double x);
typedef double (*f)(double);

double TwoPointSearch(dFunc f);
double B_Search(dFunc f, double x1, double x2, double f1, double f2);
double ratio1(double);
double ratio2(double);
double sing1(double);
double sing0(double);

double Adiff2_l(double x);
double Adiff3_l(double x);
double b_fm_Adiff2_l(double y);
double b_fm_Adiff3_l(double y);
double A1_fm_b(double x);
double b_fm_A1(double x);
double A2_fm_b(double x);

void CalcFuncMinMaxY(double (*f)(double),
                      double minX, double maxX, double *minY, double *maxY);

void MainPlotFunction(dFunc f);
double MainDoTwoPointSearch(dFunc f, int i);
void MainDoOnePointSearch(dFunc f, dFunc deriv, int searchtype);

void write_x(double *a, int n);
double tang(double A);
double Dtang(double A);
double sing(double A);
double Dsing(double A);
main()
{
    extern double W, b1, b2, a1, a2, a3, ratio21, U, G, U2-1, Ratio1, tolerance;
    double tau1, tau2, tauMin, tauMax;
    double WW, D, Dmax, Dmin, Dtest, A-norm, b-norm;
    double diff2-1, diff3-1, U3-1;
    double model, mode2, mode3, C1, C2, C3;
    double ratioMin, ratioMax, ratio31, ratio32;
    double TauTolerance, temp;
    int i, intD;
    FILE *outfile, *infile;
    char data[20], id[12];

    printf("Read data from which file? ");
    scanf("%s", data);
    infile = fopen(data, "r");
    printf("Reading in Data Parameters...
");
    fscanf(infile, "%lf %lf %lf", &model1, &mode2, &mode3); // mode1, mode2, mode3
    fscanf(infile, "%lf %lf %lf", &C1, &C2, &C3);
    fscanf(infile, "%lf %lf %lf", &W, &D, &gamm);
    fscanf(infile, "%s", id);

    strcat(data,".RM");
    outfile = fopen(data, "w");
    fprintf(outfile, "THESE ARE THE RESULTS FOR DATA %s
", id);
    fprintf(outfile, "W=%g, D=%g
", W, D);

    ratio21 = C2/C1;
    diff2-1 = mode2-model;
    WW = W*W;
    Dmax = WW*diff2-1/minU2-1;
    Dmin = WW*diff2-1/maxU2-1;

    printf("D must be in [%g,%g]
", Dmin, Dmax);
    fprintf(outfile, "D in [%g,%g]
", Dmin, Dmax);
printf("C2/C1 is \%g\n", ratio21);

/* I'm not sure what the purpose of this was */

a2 = sqrt((mode2)/D)*W;
SetBmax();
bl = b2 = Bavg;
a1 = MainDoTwoPointSearch(sing, 0);
Dtest = mode1/(a1*a1/WW);

A_norm = WW/D;   b_norm = D/W;
G = gamm*W; U2_1 = A_norm*diff2_1;
Bmin = 0.1/b_norm; Bmax = 1e6/b_norm; Bavg=(Bmax-Bmin)/2;
RatioTolerance = ratio21/100;

/****************************
...............Main Algorithm..............................................
.......................
BASIC IDEA: to use a self-consistent approach for finding b1, b2 from
(a2*a2-a1*a1) and C2/C1.

(1) Using sqrt(mode2-1/tau) as the actual a2,
    find the maximum possible B and minimum possible B.
    (The first time, tau = infinity.)
(2) Using these B values, find the extreme limits of C2/C1.
(3) Now with an assumed a2, and the limits of B and C2/C1, guess a b1 value
    (which sets b2) until you find a pair which satisfies C2/C1.
(4) Knowing an assumed b1,b2, calculate a1.
(5) Subtract D*a1*a1 from model to get a guess of the lifetime
    (which is the max possible lifetime, the first time.)
(6) Feed this lifetime back into step (1) and repeat.

CONTINUE THIS PROCESS UNTIL THE CHANGE IN LIFETIME IS NEGLIGIBLE.


/*...*/
if (D < Dmin)
    printf("D is too small\n");
else if (D > Dmax)
    printf("D is too large\n");
else{
    tauMin = 1/(mode2 - D*PI/WW);
    tau2 = tau1 = 1e100; /* infinite bulk lifetime the first time */

    for (i=1; i==1 && fabs(tau2-tau1)>TauTolerance; i++){
        tau2 = tau1;
        a2 = sqrt((mode2-1/tau2)/D)*W;
        SetBmax();
        ratioMax = (*ratio)(Bmax);
        ratioMin = (*ratio)(Bmin);
        /*while (ratioMax*ratioMin > 0.0){
            tau2 *=2;
            a2 = sqrt((mode2-1/tau2)/D)*W;
            SetBmax();
            ratioMax = (*ratio)(Bmax);
        }
        */
        switch (Choose(ratio21)){
            case 1: /* surfaces are equal, result is true */
                break;
            case 2: b1 = B_Search(ratio, Bavg, Bmax,
                ratioMin, ratioMax);
                break;
            case 3: b2 = B_Search(ratio, Bavg, Bmax,
                ratioMin, ratioMax);
                break;
            case 4:
                break;
            case 5:
                printf("Sorry, Charlie!\n");
                break;
        }
    }
\[
\text{tau} = \frac{1}{(\text{mode1} - D \cdot a1 \cdot a1 / WW)};
\]
\[
\text{TauTolerance} = \text{tau1} \times 100;
\]

\[
\text{if} \ (i == 1) \{
\]
\[
\text{tauMax} = \text{tau1};
\]
\[
\text{printf}("\text{Bulk lifetime is } \%g\text{\ h}, \text{tau1});
\]
\[
\text{fprintf}(\text{outfile}, "\text{Absolute Bulk lifetime range: }\%
\text{g}, \%g\text{\ h}, \text{tauMin, tauMax});
\]
\[
\text{fprintf}(\text{outfile}, "\text{Worst case SRVs: }\%g\text{\ h}, \text{tau2}, \text{taul});
\]
\[
\text{fprintf}(\text{outfile}, "\text{S1=\%g\ h, S2=\%g\ h,}\n\]
\[
\text{b1*b_norm, b2*b_norm});
\]
\[
\text{fprintf}(\text{outfile}, "a1*a1=\%g, a2*a2=\%g\text{\ h}, \%g\text{\ h}, \text{tau2, tau1});
\]
\[
\}
\]
\[
\text{else}\{
\]
\[
\text{printf}("\text{tau2}=\%g\text{\ h}, \text{tau2);}
\]
\[
\text{printf}("\text{tau1}=\%g\text{\ h}, \text{taul);}
\]
\[
\text{fprintf}(\text{outfile}, "\text{iteration }\%d\text{\ h}, i);\n\]
\[
\text{fprintf}(\text{outfile}, "\text{tau2=\%g\text{\ h, tau1=\%g\ h}, tau2, taul);}
\]
\[
\}
\]
\[
\text{fprintf}(\text{outfile}, "S1=\%g\text{\ h, S2=\%g\ h,}\n\]
\[
\text{b1*b_norm, b2*b_norm});
\]
\[
\text{fprintf}(\text{outfile}, "a1*a1=\%g, a2*a2=\%g\text{\ h, \%g\text{\ h,}\n\]
\[
\text{a2*a2/WW, a1*a1/WW});
\]
\]
\[
\text{/* NOW, PRINT OUT THE FLIPPED-OVER AMPLITUDE RATIO */}\n\]
\[
\text{temp = b2;}
\]
\[
\text{b2 = b1;}
\]
\[
\text{b1 = temp;}
\]
\[
\text{fprintf}(\text{outfile}, "\text{THESE ARE THE RESULTS FOR DATA }\%s\text{\ h, id);}\n\]
\[
\text{fprintf}(\text{outfile}, "\text{W=}\%g, \text{D=}\%g\text{\ h, W, D);}\n\]
\[
\text{fprintf}(\text{outfile}, "\text{C2/C1 from the original is }\%g\text{\ h, ratio21);}\n\]
\[
\text{fprintf}(\text{outfile}, "\text{C2/C1 for the opposite side should be }\%g\text{\ h, (*rat)(bl));}\n\]
\]
\[
\text{exit(0);}
\]
double A-amplit(double a){
    extern double F, G, W, b1, b2;
    double aa=a*a, bb1=b1*b1, bb2=b2*b2;
    double GG = G*G, norm, numerator;

    /* these were verified using Maple, 9/27/95 */

    /* Units of 'norm' is cm */
    norm = W/(2*aa)*( b2*(aa+bb1)/(aa+bb2) + b1 + (aa+bb1) );

    /* Units of 'F' is 1/cm^2, so 'A' has units of 1/cm^3 */
    numerator = W/(GG+aa)*(
        (G+b1)*(1 - exp(-G)*cos(a)) + exp(-G)*(a - G*b1/a)*sin(a) );

    return( gamm*F*numerator/norm );
}

double C_amplit(double a){
    extern double W, b1;
    double aa=a*a;

    /* this was verified using Maple, 9/27/95 */

    /* Since 'A' has amplitude of 1/cm^3, 'C' has amplitude of 1/cm^2 because 'B' has amplitude of cm */
    return( A_amplit(a) * W/aa*(b1*(1-cos(a)) + a*sin(a)) );

    /* if BO is greater, then amplitude ratio is positive; 
      If ratio is about zero, then assume Bs are about equal. 
      If ratio is large positive, then b0 is much larger; 
      if ratio is large negative, then b1 is much larger. 

Perhaps you can set up "b" search sectors based on the ratios. */

```c
int Choose(double ratio21){
    if (fabs(ratio21) < 1e-9)
        return(1);
    else if (ratio21 > 0.0)
        return(2);
    else if (ratio21 < 0.0)
        return(3);
}

/* 13–Search does not work unless search range is limited to positive B values. */
/* This could be avoided if the relation of B wrt the 2-1 mode difference is found */
void SetBmax()
{
    extern double Bmin, Bmax, Bavg, a2;

    Bmax = a2*(a2*tan(a2)-Bmin)/(a2+Bmin*tan(a2));
    Bavg = (Bmax-Bmin)/2;
}

double rat(double x)
{
    extern double G, a1, a2, b1, b2, W;
    double norm1, norm2, num1, num2, int1, int2;
    double aa1, aa2, bb1, bb2, GG, A1, A2, C1, C2, F=1;

    b1 = x;
    b2 = a2*(a2*tan(a2)-b1)/(a2+b1*tan(a2));
    bb1= b1*b1;
    bb2= b2*b2;
    GG = G*G;

    a1 = MainDoTwoPointSearch(sing, 0);
    aa1=a1*a1;
```
norm1 = W/(2*aa1)*( b2*(aa1+bb1)/(aa1+bb2) + b1 + (aa1+bb1));
num1 = W/(GG+aa1)*
       (G+b1)*(1-exp(-G)*cos(al)) +exp(-G)*(a1-G*b1/a1)*sin(al));
  
A1 = gamm*F*num1/norm1;
int1 = W/aa1*(b1*(1-cos(al)) + a1*sin(al));
C1 = A1*int1;

a2 = MainDoTwoPointSearch(sing, 1);
aa2=a2*a2;

norm2 = W/(2*aa2)*(b2*(aa2+bb1)/(aa2+bb2) + b1 + (aa2+bb1) );
num2 = W/(GG+aa2)*
       (G+b1)*(1-exp(-G)*cos(a2))+exp(-G)*(a2-G*b1/a2)*sin(a2));

A2 = gamm*F*num2/norm2;
int2 = W/aa2*(b1*(1-cos(a2)) + a2*sin(a2));

C2 = A2*int2;

 return(C2/C1);
}

double ratio(double x)
{
 extern double G, a1, a2, b1, b2, ratio21;
 double test-ratio;

 /* knowing a2, and having chosen b0 makes b1 and a1 known quantities */

test-ratio = rat(x);
 printf( "(b1,b2)=(%g,%g)\t a1=%g\n", b1, b2, a1);
 printf("t C2/C1 is %g\n", test-ratio);
 if (ratio21 > 0.0)
 return(ratio21 - test-ratio);
 else
 return(ratio21 + test-ratio);
double diff() {
    extern double b1, b2, U2-1;
    double b_avg = (b1+b2)/2;
    double a2, a1;

    a1 = MainDoTwoPointSearch(sing,0);
    a2 = MainDoTwoPointSearch(sing,1);
    return( U2_1 - 2*b_avg*(a2/tan(a2) - a1/tan(a1)) );
}

double sing(double A) {
    extern double b1, b2;

    return( (A*A-b1*b2)*sin(A) - A*(b1+b2)*cos(A) );
}

double equal(double b) {
    extern double a2;

    return( (a2*a2-b*b)*sin(a2) - a2*2*b*cos(a2) );
}

double sing2(double x) {
    extern double a2, b2;
    double B2 = b2, B1 = x;

    return( (a2*a2-B1*B2)*sin(a2) - a2*(B1+B2)*cos(a2) );
}

double sing1(double x) {
extern double a1, b2;
double B2 = b2, B1 = x;
return( (a1*a1-B1*B2)*sin(a1) - a1*(B1+B2)*cos(a1));
}

double B_Search(dFunc f, double x1, double x2, double f1, double f2)
{
    int count;
double minY, maxY, rootGuess, step;
extern double RatioTolerance;
double xMiddle, fGuess;

    step = (x2-x1)/3;
    rootGuess = x2;
    fGuess = f2;
    while( (f1<0 & & fGuess>0) || (f1>0 & & fGuess<0) ){
        rootGuess -= step; /*...step downward */
        fGuess = (*f)(rootGuess);
    }
    x1 = rootGuess;
    x2 = rootGuess + step;

    for(count=0; fabs(fGuess) > RatioTolerance; count++){
        xMiddle = (x1+x2)/2;
        fGuess = (*f)(xMiddle);
        if( (f1<0 & & fGuess>0) || (f1>0 & & fGuess<0) ){
            x2 = xMiddle;
            f2 = fGuess;
        }
        else {
            x1 = xMiddle;
            f1 = fGuess;
        }
    }
    rootGuess = x1 + f1*(x1-x2)/(f2-f1);
double MainDoTwoPointSearch(dFunc f, int i)
{
  int count;
  double x1, x2, rootGuess, xMid;
  double minY, maxY, f1, f2, fMid;
  const double tolerance = le-6;
  
  x1 = (i)*PI;
  if (i == 0)
    x1 = le-2;
  x2 = (i+1)*PI;
  CalcFuncMinMaxY(f, x1, x2, &minY, &maxY);
  
  /* You vary the thing you're looking for, until you find it */
  f1 = (*f)(x1);
  f2 = (*f)(x2);
  rootGuess = f1*(x1-x2)/(f2-f1) + x1;
  
  for(count=0; fabs((*f)(rootGuess)) > tolerance; count++) {
    xMid = (x1+x2)/2;
    fMid = (*f)(xMid);
    if(( f1<0 & & fMid>0) || (f1>0 & & fMid<0)) {
      x2 = xMid;
      f2 = fMid;
    }
    else{
      x1 = xMid;
      f1 = fMid;
    }
  }

  fGuess = (*f)(rootGuess);
  return(rootGuess);
}
void CalcFuncMinMaxY(double (*f)(double), double minX, double maxX, double *minY, double *maxY)
{
    double x, y, step;
    *minY = 0;  *maxY = 0;
    step = (maxX-minX) / StepNum;
    for(x = minX; x <= maxX + step/2; x += step) {
        y = (*f)(x);
        if( y < *minY )
            *minY = y;
        else if(y > *maxY)
            *maxY = y;
    }
}
Appendix D: Computer Codes Used In Theoretical Studies Of Microwave Detection

D. Microwave reflectance from multilayered media

c:..............................................
c program: planewave multilayer reflection
c author: Frederick P. Giles
c date: 12/10/92
c version: 1.2
c purpose: Calculate Oblique incidence

c 1-D transmission and reflection coefficients for

c plane waves in multiple planar layers of

c  general media.

c Program should be adaptable to

c transmission lines, and wave functions.

c For sinusoidal steady state, i.e., complex exponentials,

c this is the solution at a boundary

c of a differential equation

c as a constant coefficient changes.

c:..............................................

program oblique multilayer reflection
Constants Declarations

c note: these are the "per centimeter" values

integer LAYERS
parameter (LAYERS=10)
real EPSO, MUO, DBLPI, ETAO, C, PI
parameter (EPSO=8.854187818e-14, MUO=12.5663706144.e-9)
parameter (DBLPI=6.283185307, ETAO=376.7303138)

real OneRadian
parameter (OneRadian=57.2957795)

Variables Declarations

complex rho, eps(LAYERS), Zload, Zin, ZO(LAYERS)
complex kl(LAYERS), index(LAYERS), cplxtrans
integer i, numoflayers, mode, keylayer
real hzfreq, radfreq, k0, epsrel, sigma, thickness
real rhoabs, reflpower, cutofffreq
real theta(LAYERS), sigmaSteps, sigmaIncr
real keyeps, keythickness, tangential, normal

Subroutine Declarations

external Smithchart, SmallAngle
complex SmithChart
real SmallAngle

write(6,*) "One part of this program is faulty:"
write(6,*) "the computed angles don't allow for complex indices."
write(6,*) "............................................"
write(6,*) 'program: oblique_refl2.1.f"
write(6,*) "computes reflections for plane waves of any angle"
write(6,*) " of incidence "
write(6,*) "data was read from (oblique_refl2.1.data)"
write(6,*) "This version auto-varies conductivity values   "
write(6,*) "---------------------------------------------"

!READ IN PARAMETERS AND DATA

open (unit=1, file="oblique_refl2.1.data")
rewind 1
read(1,*) numoflayers
read(1,*) hzfreq
read(1,*) cutofffreq
read(1,*) mode
read(1,*) keylayer
read(1,*) sigmaSteps
read(1,*) sigmaincr

!CIOMPUTE WAVE PARAMETERS FOR EACH LAYER

radfreq = DBLPI*hzfreq
k0 = radfreq/C

!READ IN THE PARAMETERS FOR EACH LAYER, COMPUTE WAVEPARAMS

do 10 i=1,numoflayers,1
   read(1,*) epsrel, sigma, thickness
   if (i.eq.keylayer) then
      keyeps = epsrel
      keythickness = thickness
   endif
10 continue
eps(i) = cmplx(EPS0*epsrel, -sigma/radfreq)

index(i) = ccsqrt(eps(i)/EPS0)

kl(i) = k0 * index(i) * thickness

write(6,*), "eps is ", eps(i)

write(6,*), "kl is ", kl(i)

continue

c:........................................................................
c COMPUTE INCIDENT ANGLE AND IMPEDANCE OF FIRST LAYER

c:........................................................................

theta(1) = asin( sqrt(1 - (cutofffreq**2/hzfreq**2)) )

if (mode.eq.0) then
   ZO(1) = ccsqrt(MU0/eps(1))/cos(theta(1))
else
   ZO(1) = ccsqrt(MU0/eps(1))*cos(theta(1))

endif

c:........................................................................
c Main Calculations Loop

c:........................................................................
c Definitions:
c 'ZO is the intrinsic E-M impedance of a medium
c 'Zin is total impedance following, a distance in front of a boundary
c 'Zload is total impedance following, from the edge of a boundary

c:........................................................................

open(unit=2, file="r")
rewind 2
open(unit=3, file="sigma")
rewind 3
open(unit=4, file="refl")
rewind 4

c:........................................................................
c RE-COMPUTE PARAMETERS FOR THE KEY LAYER, FOR ITERATIONS

\[
\begin{align*}
do 161 = 0, & \text{sigmaSteps,} l \\
\text{sigma} = l * \text{sigmaIncr} \\
\text{eps(keylayer)} = \text{cmplx(EPS0*keyeps, -sigma/radfreq)} \\
\text{index(keylayer)} = \text{csqrt(eps(keylayer)/EPS0)} \\
\text{kl(keylayer)} = kO * \text{index(keylayer)} * \text{keythickness}
\end{align*}
\]

\[
\begin{align*}
\text{c COMPUTE TRANSMITTED ANGLES USING SNELL'S LAW} \\
\text{c See Stratton, Electromagnetic Theory, p. 501-502}
\end{align*}
\]

\[
\begin{align*}
do 15 & \text{i=}2,\text{numoflayers,} l \\
\text{if (i.eq.keylayer) then} \\
\text{c This is indeed the cplx cosine of the transmitted part, by Snell's law} \\
\text{cplxtrans} = \text{csqrt(1 - (index(i-1)/index(i))**2 * sin(theta(i-1))**2)} \\
\text{c This is the real part of the incident tangential component,} \\
\text{c which must be continuous at the interface (same in the trans. medium)} \\
\text{tangential} = \text{real(index(i-1)*cplxtrans (i))} \\
\text{c This is the transmitted normal component, "q"} \\
\text{normal} = \text{real(index(i)*cplxtrans)} \\
\text{theta(i)} = \text{asin(tangential/sqrt(tangential**2 + normal**2))} \\
\text{elseif (i.eq.keylayer+1) then} \\
\text{theta(i)} = \text{theta(1)} \\
\text{else} \\
\text{c This is only good for real indices (lossless materials)} \\
\text{theta(i)} = \text{asin(real(index(i-1)/index(i))*sin(theta(i-1)))} \\
\text{endif}
\end{align*}
\]

\[
\begin{align*}
\text{c} & \text{ write(6,*), "tangential is", tangential} \\
\text{c} & \text{ write(6,*), "normal is", normal} \\
\text{c} & \text{ write(6,*), "theta(*,i,\) is", theta(i)*OneRadian}
\end{align*}
\]
if (mode.eq.0) then
   \( Z_0(i) = \frac{\text{csqrt}(\mu_0/\varepsilon(i))}{\cos(\theta(i))} \)
else
   \( Z_0(i) = \text{csqrt}(\mu_0/\varepsilon(i)) \times \cos(\theta(i)) \)
endif

continue

--------------------------------------------------------

\text{c COMPUTE IMPEDANCES OF LAYERS, TRANSFORMING THEM BACK}
--------------------------------------------------------

\( Z_{\text{load}} = Z_0(\text{numoflayers}) \)

do 20 i = \text{numoflayers}-1, 2, -1
   \( Z_{\text{in}} = \text{SmithChart}(Z_{\text{load}}, Z_0(i), \kappa(i)) \)
   \( Z_{\text{load}} = Z_{\text{in}} \)
   write(6,*), "Z_{\text{in}} is ", Z_{\text{in}}
20 continue

write(6,*), "Z_{\text{load}} is ", Z_{\text{load}}

\( \rho = \frac{(Z_{\text{load}} - Z_0(1))}{(Z_{\text{load}} + Z_0(1))} \)
\( \rho_{\text{abs}} = \text{cabs}(\rho) \)
\( \text{reflpower} = \rho_{\text{abs}} \times \rho_{\text{abs}} \)

write(6,*), "reflected power is"
write(2,*), sigma, " reflpower ", reflpower
write(3,*), sigma
write(4,*), reflpower

continue

close(unit=2)
close(unit=3)
close(unit=4)
c Reduct real angles to less than 2 PI

real function SmallAngle(kl)

real kl
real DBLPI
parameter (DBLPI=6.283185307)

SmallAngle = mod(kl, DBLPI)
end

c Smith Chart transformation

complex function SmithChart(Zload, ZO, kl)

complex Zload, ZO, kl
complex j
parameter (j = (0,0,1.0))

SmithChart = Z0*(Zload*ccos(kl) + j*ZO*csin(kl)) /
~ (ZO*ccos(kl) + j*Zload*csin(kl))
end
D.2 Dependence of microwave reflectance upon excitation spot size

program: reflectance calculations
author: Frederick P. Giles
date: 10/20/92
version: 1.0
purpose: To calculate normal incidence transmission and reflection coefficient for transmission lines, plane waves, and quantum waves.

program circles of reflectance

Clonstant
integer AREAS, SIGMAS
parameter (AREAS=7, SIGMAS=25)
real EPSO, MUO, DBLPI, ETAO, C, PI
parameter (EPSO=8.854e-14, MUO=1.256e-8, DBLPI=6.283185, ETAO=377, C=3e10, PI=3.141592654)
these are the "per centimeter" values

Variables
real sigma(SIGMAS), hzfreq, radfreq, sigma0, area0,
area(AREAS), rhoabs0, rhotot(AREAS,SIGMAS),
rhoabs(sigma0), reflpowertot(AREAS,SIGMAS),
reflpower0, reflpower(sigma0), sig,
skindepth(SIGMAS), Drhotot(AREAS,SIGMAS),
Dreflpowertot(AREAS,SIGMAS)
complex csinh, ccosh, Zload, rho
integer i, j, numofareas, numofsigma
intrinsic ccos, csin, exp, sinh, cosh, csqrt, cmplx, cexp, cabs
external csinh, ccosh

:::---------------------------------
 External Data Read-in

:::---------------------------------
C:---------------------------------------------------------------------
  open (unit=1, file="circle.data")
  rewind 1
  open (unit=2, file="sigma")
  rewind 2
  open (unit=8, file="area")
  rewind 8
  read(1,*) hzfreq
  read(1,*) sigma0
  read(1,*) area0
  read(1,*) numofareas
  read(1,*) numofsigma
  write(8,*) "0.0"
  write(2,*) "0.0"

  do 10 i=1,numofareas,1
    area(i) = real(i)/real(numofareas)*area0
    write(8,*) area(i)/area0
  10
  do 11 i=1,numofsigma,1
    sigma(i) = real(i)/real(numofsigma)*sigma0
    write(2,*) sigma(i)/sigma0

  close (unit=1)
  close (unit=2)
  close (unit=8)

  radfreq = DBLP1*hzfreq
  eta = ETA0

  open (unit=9, file="skindepth")
  rewind 9

C:---------------------------------------------------------------------
  c Calculate the Background Reflectivity
Zload = csqrt(MU0 / cmplx( EPS0*11.7, sigma0/radfreq ))  

rho = (Zload - eta)/(Zload + eta)  
rhoabs0 = cabs(rho)  
reflpower0 = rhoabs0*rhoabs0  
skindepth0 = 1/sqrt(PI*hzfreq*MU0*sigma0)  
write(9,*) skindepth0*1e4  

rhoabs(i) = cabs(rho)  
reflpower(i) = rhoabs(i)*rhoabs(i)  
skindepth(i) = 1/sqrt(PI*hzfreq*MU0*sig)  
write(9,*) skindepth(i)*1e4  

continue

5  continue

close (unit=9)

c Open the files to place output data into

c
open (unit=1,file="area1")  
rewind 1  
open (unit=2,file="area2")  
rewind 2

Calculations for Photoconductivity Reflectivity

Calculations for Photoconductivity Reflectivity
open (unit=3,file="area3")
rewind 3
open (unit=4,file="area4")
rewind 4
open (unit=5,file="area5")
rewind 5
open (unit=8,file="area6")
rewind 8
open (unit=9,file="area7")
rewind 9

c::: Calculation of Net Reflectivity and Skindepths

c::: Calculation of Net Reflectivity and Skindepths

write(1,*) rhoabsO
write(2,*) rhoabsO
write(3,*) rhoabsO
write(4,*) rhoabsO
write(5,*) rhoabsO
write(8,*) rhoabsO
write(9,*) rhoabsO

do 15 j=1,numofareas
do 20 i=1, numofsigea
    rhotot(j,i) = rhoabs0*(area0 - area(j))/area0
    - + rhoabs(i)* (area(j)/area0)

    if (j.eq.1) then
        write(1,*) rhotot(j,i)
    elseif (j.eq.2) then
        write(2,*) rhotot(j,i)
    elseif (j.eq.3) then
        write(3,*) rhotot(j,i)
    elseif (j.eq.4) then

write(4,*), rhotot(j,i)
elseif (j.eq.5) then
    write(5,*), rhotot(j,i)
elseif (j.eq.6) then
    write(8,*), rhotot(j,i)
elseif (j.eq.7) then
    write(9,*), rhotot(j,i)
endif

Drhotot(j,i) = (rhotot(j,i) - rhoabs0)/rhoabs0
write(1,*), Drhotot(j,i)
reflpowertot(j,i) = rhotot(j,i)*rhotot(j,i)
Dreflpowertot(j,i) = (reflpowertot(j,i) - reflpower0)/C-
write(3,*), Dreflpowertot(j,i)

continue
continue

close (unit=1)
close (unit=2)
close (unit=3)
close (unit=4)
close (unit=5)
close (unit=8)
close (unit=9)

stop
end