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## Semiconductor Measurement Technology:

## A FORTRAN Program for Galculating the Electrical Parameters of Extilisic Sillicon

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# A FORTRAN Program for Calculating the Electrical Parameters of Extrinsic Silicon 

R. D. Larrabee, W. R. Thurber, and

W. M. Bullis

Electron Devices Division<br>Center for Electronics and Electrical Engineering<br>National Engineering Laboratory<br>National Bureau of Standards<br>Washington, DC 20234


U.S. DEPARTMENT OF COMMERCE, Philip M. Klutznick, Secretary

Luther H. Hodges, Jr., Deputy Secretary
Jordan J. Baruch, Assistant Secretary for Productivity, Technology and Innovation NATIONAL BUREAU OF STANDARDS, Ernest Ambler, Director

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Page
Abstract ..... 1

1. Introduction ..... 1
2. Description of Program Operation ..... 3
2.1 Options ..... 5
2.1.1 DOUBLE ON ..... 5
2.1.2 DOUble off ..... 6
2.1.3 CONSTANTS ..... 6
2.1.4 DOLOOP XX ARG(1) ARG(2) ..... 7
2.1.5 STOP ..... 8
2.2 Warning and Error Messages ..... 8
2.3 Additional Information ..... 9
3. Theory and Method of Computation ..... 10
3.1 Location of the Fermi Level ..... 10
3.2 Computation of Carrier Mobilities and Related Parameters ..... 14
4. Annotated Program Listing ..... 19
5. Illustrative Output Data Cards and Examples ..... 36
5.1 Data Cards Used to Generate Output Listings ..... 36
5.2 Illustration of a No-Option Output ..... 37
5.3 Illustration of the DOUBLE ON Option Output ..... 38
5.4 Illustration of the DOLOOP XX Option Output ..... 41
5.5 Illustration of the CONSTANTS Option Output ..... 45
6. Conclusions ..... 46
Acknowledgments ..... 46
References ..... 46
List of Tables
Page
7. Symbols Used in Mobility Formulas ..... 15
8. Formulas for Calculating Electron Mobility ..... 16
9. Formulas for Calculating Hole Mobility ..... 17

The computer program described in this report evolved during the course of a number of projects in the Semiconductor Technology Program in the Electron Devices Division at the National Bureau of Standards. This program serves to focus NBS efforts to enhance the performance, interchangeability, and reliability of discrete semiconductor devices and integrated circuits through improvements in measurement technology for use in specifying materials and devices in national and international commerce for use by industry in controlling device fabrication processes. Its major thrusts are the development of carefully evaluated and well-documented test procedures and associated technology and the dissemination of such information to the electronics community.

A FORTRAN Program for Calculating the Electrical Parameters of Extrinsic Silicon

## by

R. D. Larrabee, W. R. Thurber, and W. M. Bullis National Bureau of Standards Washington, DC 20234


#### Abstract

Many electrical properties of silicon are strongly dependent upon the specific nature and density of the active impurities present. Calculation of these electrical properties hinges on the solution of the charge balance equation to determine the position of the Fermi level for each specific case of interest. A FORTRAN program is presented that performs this determination and then calculates some of the often-used electrical parameters of silicon as a function of temperature. Results obtained from this program have proven useful in interpreting Hall effect data, determining the degree of ionization of the separate dopant states as a function of temperature, predicting the behavior of specimens when the dopant picture is intentionally (or conceptually) changed, and understanding the variations in the relative roles of the different scattering mechanisms on carrier mobility as the temperature is changed.


Key Words: Carrier density; computer program; electri- cal properties of silicon; Hall effect; mobility; resistivity; silicon.

## 1. INTRODUCTION

Trace impurities can act as donors or acceptors and thus contribute mobile charge carriers that can have a profound effect on resistivity and other electrical properties. Since carrier density and mobility are functions of temperature as well as the density and type of impurities present, it is impractical to provide general tables listing all possible situations that might occur in practice. Therefore, it becomes necessary to calculate the desired electrical properties for each impurity situation and temperature of interest.

The FORTRAN program presented in this report was written to accomplish this objective for the case of simple donor and acceptor states in silicon (hereafter called dopant states). The density, activation energy, and degeneracy of all active donors and acceptors are initially provided as inputs to the program. These data are then used by the program to calculate the position of the Fermi level by solving the detailed charge balance equation (i.e., the sum of the positive charges in the valence band and ionized donors equals the sum of negative charges in the conduction band and ionized acceptors). After
the position of the Fermi level has been found, the program computes many of the more often used electrical properties of silicon that depend on carrier density or carrier scattering (e.g., resistivity, carrier mobility, and Hall coefficient). The scattering mechanisms which are included in the calculation of the carrier mobility are lattice, ionized impurity, neutral impurity, and electron-electron (or hole-hole) interactions. Both electron and hole mobilities are calculated and an effective conductivity mobility is calculated as the sum of the electron and hole mobilities weighted by the density of each. The effective conductivity mobility computed this way is the same as the majority carrier conductivity mobility in extrinsic specimens. In intrinsic specimens, it corresponds to a hypothetical mobility for the total carrier density (i.e., electron plus hole density). The expressions for calculating the resistivity and Hall coefficient include appropriately weighted contributions from both charge carriers. In the absence of agreement as to appropriate values, the Hall scattering factors (i.e., ratio of Hall to conductivity mobility) for both electrons and holes were taken to be unity.

In its present form, the program handles up to five independent impurity states, two donors and three acceptors. The donor levels are assumed to be neutral when occupied by an electron and to have a temperature-independent activation energy referenced to the conduction band edge. The acceptor levels are assumed to be neutral when occupied by a hole and to have a temperature-independent activation energy referenced to the valence band edge. Provision is made for the reduction in activation energy for both donors and acceptors at the higher dopant densities. These assumptions are appropriate for impurities from column 3 and 5 of the periodic table (e.g., boron and phosphorus) and may, or may not, be appropriate for other impurities with larger activation energies or multiple energy levels.

The key algorithms in this program are the routine for calculating the position of the Fermi level and the routine for calculating the carrier mobilities. These algorithms are most accurate over the temperature interval from 100 to 500 K and for total doping densities below $10^{18} \mathrm{~cm}^{-3}$. These two algorithms have been written as subroutines in the present program so that they can be used as a starting point in the development of other programs that require these algorithms. Notice, however, that the mobility routine requires knowledge of many of the parameters calculated by the Fermi level routine, and thus it cannot be used without first executing the Fermi level routine.

Variations of the present program have proven useful for interpreting Hall data [1], predicting the electrical behavior when the dopant picture (e.g., compensation) is changed $[2,3]$, determining the degree of ionization of the active dopant state in extrinsic infrared detectors [4], and understanding the changing role of the various scattering mechanisms on mobility as the temperature or dopant density changes.

The following section provides the information necessary to use the program. Section 3 describes the various equations used in the program so that the interested user may verify that they are appropriate for his particular application. A detailed listing of the complete program is given in section 4. This listing is heavily annotated so that the user can identify each equation
and follow each step of the program. Section 5 provides examples of typical output formats.

## 2. DESCRIPTION OF PROGRAM OPERATION

The present program can be divided into four main parts as follows:

1. Read data cards and set up options.
2. Compute position of the Fermi level, occupancy of all dopant states, and density of carriers in the conduction and valence bands.
3. Compute carrier mobilities and related parameters.
4. Print output listings and reinitialize for next run.

In its present form, the program can handle up to two donor states (called Dl and D2) and up to three acceptor states (called A1, A2, and A3). For each dopant state, the program expects to find a data card specifying:

1. the name of the dopant state (up to 12 alphanumeric characters),
2. the density of the dopant state in reciprocal cubic centimeters,
3. the activation energy of the dopant state at infinite dilution in electron volts,* and
4. the degeneracy of the dopant state (an integer > unity).

The format of these data cards is 2A6, El0.4, 2 F10.4, corresponding to the four items of input data - name, density, activation energy, and degeneracy, respectively. The format for the name (2A6) assumes that the machine can store 12 alphanumeric characters in two 6 -character words. This may have to be changed for machines with different alphanumeric storage formats. If a particular dopant state is absent, its data card must still be present to inform the program of this fact. The data cards representing missing dopant states use the name DUMMY and the rest of the card is left blank. The order of the five data cards is:

1. Dl - first donor state,
2. D2 - second donor state,
3. Al - first acceptor state,
4. A2 - second acceptor state, and
5. A3 - third acceptor state.

It is recommended that this same order (i.e., Dl through A3) be the order of occurrence of the corresponding dopant states from the conduction band to the valence band (if possible) to aid in remembering which symbol (i.e., Dl through A3) represents each dopant state.
*For donor states, the activation energy is the magnitude of the energy difference between the conduction band and the dopant state; for acceptor states, it is the magnitude of the energy difference between the valence band edge and the dopant state. Both of these quantities are assumed to be independent of temperature.

In the normal (no-option) output format, the program lists the following quantities on the output page for each set of five input data cards supplied:

1. the position of the Fermi level with respect to the valence band in electron volts,
2. the density of electrons in the conduction band in reciprocal cubic centimeters,
3. the density of holes in the valence band in reciprocal cubic centimeters,
4. the effective conductivity mobility in square centimeters per volt-second,
5. the Hall coefficient in cubic centimeters per coulomb,
6. the electrical resistivity in ohm-centimeters, and
7. the ionized density of dopant species D1 through A2 in reciprocal cubic centimeters. (The DOUBLE ON option discussed below can be used to output the ionized density of species A3.)

These ten items are printed across a single line on the output listing in the order given. Since these parameters are functions of temperature, the output listing consists of a series of such lines, each preceded by its temperature and the corresponding value of $1000 / T$. The resulting table is provided with descriptive column headings and documentation of the appropriate input information from the data cards (see first sample output listing in sec. 5). The program is capable of listing additional output information, as discussed in the section on options to follow.

The above quantities are evaluated and listed as a function of temperature over the range from 4.2 to 500 K . This temperature range is divided into three regions, with break-points at 77 K (liquid nitrogen temperature) and 300 K (room temperature). The program will perform its evaluations at each break-point (i.e., 77 and 300 K ), as well as at the extreme points (i.e., 4.2 and 500 K ). After completion of the first evaluation at 4.2 K , the program jumps to some higher specified temperature and then starts to increase the temperature with equal increments of $1000 /(t e m p e r a t u r e)$. The incremental values of $1000 /(t e m p e r a t u r e)$ are specified independently in each of the three temperature regions. As presently written, the temperature following 4.2 K is $20 \mathrm{~K}(1000 / \mathrm{T}=50)$, and then the temperature is increased in intervals of $1000 / T=2$ until the first break-point at 77 K is reached. Within the interval from 77 K to 300 K , the temperature is increased in intervals of $1000 / \mathrm{T}=$ 1. Above 300 K , the temperature is increased in intervals of $1000 / \mathrm{T}=0.5$. The FORTRAN parameter RUNNO keeps track of things as follows:

```
RUNNO = l, first time through, T = 4.2 K,
RUNNO = 2, first region up to 77 K,
RUNNO = 3, second region from 77 to 300 K, and
RUNNO = 4, third region above 300 K.
```

Many of these details of the temperature sequence can easily be changed by simply changing the appropriate defining statements in the program (e.g., the first temperature of 4.2 K is defined by the FORTRAN statement numbered 170 in the program listing in sec. 4.).

Several options are built into this program to allow one to modify the output listing without changing the program per se. These options are exercised when a control card is inserted into the data card deck so that it is read by the program as a D1 data card. The program recognizes that it is a control card and not a D1 data card by the name. When such a control card is encountered, the program sets up the option desired and then goes back and expects the next card to be a D1 data card. If no control cards are included in the deck of input data cards, the program simply generates an output listing as outlined previously.

This is considered to be the normal (or no-option) output format and is the format that should suffice for most applications of this program.

The control cards consist of a single (or double) word name selected from a reserved name list designed not to conflict with dopant state names. Some of the control cards additionally contain numerical arguments that are needed to specify the parameters of the option desired. In either event, the format of all control cards is identical to that of the dopant state data cards (i.e.. 2A6, El0.4, 2Flo.4), so the names and any numerical arguments must be placed on the control card accordingly.
2.1.1 DOUBLE ON

This option doubles the amount of data printed on the output listing at each temperature. The format of the output listing consists of two lines of output information at each temperature instead of just one (thus the name DOUBLE ON). The first line of information is identical to a no-option run* and the second line contains the parameters listed below. The corresponding control card consists of the two words DOUBLE $O N$ in the first nine positions with the rest of the card blank. This control card turns on this option for all subsequent sets of dopant state data cards, and it remains on until a DOUBLE OFF control card is read. This means that the DOUBLE ON control card must be the first card of a group of data card sets for which the double output is desired. The DOUBLE OFF control card must be the card which follows the last data card in the group (i.e., the first card of a run for which single output only is desired). In addition to all the parameters listed in a nooption run, the DOUBLE ON option will cause the program to list the following parameters:

1. The energy gap of silicon in electron volts.
2. A parameter called TEST which indicates how close the calculated Fermi level position comes to solving the detailed charge balance equation. TEST is the number of residual charges per cubic centimeter.
3. The voltage equivalent of the temperature in volts (i.e., kT/q).
4. The position of the Fermi level with respect to the conduction band in electron volts.

[^1]5. The ionized density of the dopant state A3 in reciprocal cubic centimeters (there was insufficient room for this to be included on the single-line no-option listing).
6. The electrical conductivity in mho per centimeter.
7. The mobility of electrons in the conduction band in square centimeters per volt-second, as follows:
A. the upper limiting mobility of electrons set by lattice and electron-electron scattering,
B. the mobility obtained by adding the effects of ionized impurity scattering (corrected for electron-electron scattering) to $A$, above, and
C. the mobility obtained by adding the effects of neutral impurity scattering to $B$, above.
8. The mobility of holes in the valence band in square centimeters per volt-second as follows:
A. the upper limiting mobility of holes set by lattice and holehole scattering,
B. the mobility obtained by adding the effects of ionized impurity scattering (corrected for hole-hole scattering) to A, above, and
C. the mobility obtained by adding the effects of neutral impurity scattering to $B$, above.

These parameters were selected to complement the parameters of a nooption run and are listed on the line immediately below them on the output listing, as shown in section 5.3. The sets of two-line data corresponding to each temperature are separated by two blank lines in order to make it more obvious which of the two column headings applies to each line. Some of the parameters listed here are also listed in the CONSTANTS option discussed below, and some are modified versions of parameters listed in the no-option listing (e.g., the position of the Fermi level with respect to the conduction band instead of with respect to the valence band). The three mobility values listed for electrons and holes provide information needed for giving one a picture of the changing role of the various scattering mechanisms with temperature. Although the majority carrier mobility is calculated as accurately as possible, less attention has been paid to the calculation of minority carrier mobility. (See sec. 3.2 below.)

### 2.1.2 DOUBLE OFF

This control card turns off the DOUBLE ON option as explained above. The control cards DOUBLE ON and DOUBLE OFF simply set and clear a switch, respectively, and affect nothing but the format of the output listing. Therefore, it is permissible to use any of the other control card options while in the DOUBLE ON mode of output listing. The default condition (i.e., if neither DOUBLE ON nor DOUBLE OFF control cards appear in the deck of data cards) is DOUBLE OFF.

### 2.1.3 CONSTANTS

This option generates a listing of some of the parameters used in the evaluation that are not functions of dopant density. These parameters
are evaluated at the same temperatures as a no-option run. The corresponding control card consists of the single word CONSTANTS in the first nine positions with the rest of the card blank. The CONSTANTS option does not relate in any way to any dopant state data cards that might follow. Consequently, the next card could be another control card or the D1 data card of another run. The CONSTANTS control card can be located anywhere in the deck of cards to be read by the program as long as it is encountered when the program expects to find a D1 data card. The CONSTANTS control card causes the program to list the following parameters:

1. $1000 /(t e m p e r a t u r e) ~ i n ~ i n v e r s e ~ k e l v i n, ~$
2. the temperature in kelvin,
3. the voltage equivalent of the temperature in volts (i.e., kT/q),
4. the band gap in silicon in electron volts,
5. the relative dielectric constant of silicon,
6. the upper limiting mobility of electrons in the conduction band set by lattice scattering in square centimeters per volt-second,
7. the upper limiting mobility of holes in the valence band set by lattice scattering in square centimeters per volt-second,
8. the temperature in kelvin raised to the $3 / 2$ power,
9. the relative effective mass of electrons in the conduction band,
10. the relative effective mass of holes in the valence band,
11. the density of states in the conduction band in reciprocal cubic centimeters (designated FNC in Program and on output listings), and
12. the density of states in the valence band in reciprocal cubic centimeters (designated FNV in Program and on output listings).

These parameters are printed across a single line on the output listing in the order given. Since these parameters are functions of temperature, each such line corresponds to a different temperature. The resulting table is provided with descriptive column headings as shown in the sample output listing in section 5.5. The last five items on the above list are useful for interpreting Arrhenius plots of the logarithm of carrier density vs. $1000 / T$ in terms of the activation energies of the dopant states present (e.g., as might be done in interpreting the results of measurements of Hall coefficient as a function of temperature).
2.1.4 DOLOOP XX ARG(1) ARG(2)

This option causes the program to generate multiple listings for a single set of five dopant state data cards. Each successive listing has the density of a selected dopant state incremented by a specified amount. The following information must be provided on the DOLOOP xx control card:
A. DOLOOP XX is the name; XX specifies which dopant state is to have its density incremented. XX is selected from the list D1, D2, Al, A2, and A3. If anything else appears in the $X X$ position on this control card, an error message to this effect will be printed on the output listing, and the DOLOOP XX control card will be ignored.
B. ARG(l) is a numerical argument which specifies the amount by which one would like to increase (or decrease) the dopant density each time. Its dimensions are (centimeters) ${ }^{-3}$. In accordance with the format statement pertaining to data cards (i.e., 2A6, El0.4, 2 Flo.4), it is expressed in $E$ format in positions 13 to 22 on the control card.
C. ARG(2) is a dimensionless argument which specifies the total number of listings desired. In accordance with the format statement pertaining to data cards, it is expressed in $F$ format (with decimal point) in positions 23 to 32 on the control card.

The DOLOOP XX option refers only to the next set of five dopant state data cards, and everything reverts back after completing the number of listings specified. Only one dopant state can be incremented at a time (i.e., no provision has been made for nested doloops).

### 2.1.5 STOP

This option causes a FORTRAN stop instruction to be executed and is used to exit the program. The corresponding control card consists of the single word STOP in the first four positions on the card with the rest of the card blank. Normally, the STOP control card is the last card in the deck of cards to be read by the program.

## 2. 2 WARNING AND ERROR MESSAGES

There are several warning and error messages that are printed on the output listing when unusual circumstances are encountered during the execution of the program. A warning message informs the user that the indicated condition was encountered and suggests that its effects on the validity of the next data line(s) be considered. Error messages inform the user of an event that precludes the continuation of the current run and, after printing the error message, the program proceeds to the next set of five dopant state data cards. The messages are:

1. BORN APPROXIMATION FOR IONIZED SCATTERING NOT VALID FOR MAJORITY CARRIER

This warning message is printed when the $\log$ term, $B N$, in the modified Brooks-Herring ionized impurity formula is less than or equal to 10.0 . In the Born approximation, the scattering is treated as a small perturbation on the motion of the incident carrier. This assumption is violated at high carrier densities and low temperatures.
2. (EF-EG)/CAYT $=\mathrm{XX}$ ERROR IN N MAY EXCEED 1 PERCENT

In this warning message, $X X$ is replaced by the dimensionless ratio of the difference in energy between the Fermi level and the conduction band divided by the voltage equivalent of the temperature (i.e., kT/q). This message is printed when $X X>-2$ and is a warning that the calculation of electron density may be in error by greater than 1 percent due to the expressions used to approximate the Fermi-Dirac integral [5]. This occurs only at high dopant densities when the material is degenerate or nearly so.
3. EF/CAYT $=X X$ ERROR IN P MAY EXCEED 1 PERCENT

This warning message is identical in function to that of the one immediately preceding, except that it pertains to hole density instead of electron density.
4. INVALID ARGUMENT OF DOLOOP COMMAND

This error message is printed when the argument on the DOLOOP XX control card (i.e., XX) is not selected from the list D1, D2, A1, A2, or A3. After printing this message, the program proceeds to process the run without the DOLOOP option (i.e., it produces one run instead of the number called for on the invalid DOLOOP XX control card).
5. CHARGE BALANCE EQUATION COULD NOT BE SOLVED, IFLAG $=\mathrm{X}$

This error message is printed when the algorithm for the determination of the Fermi level position cannot find a solution to the charge balance equation. When this message is printed, $X$ is replaced by the value of an integer flag (i.e., IFLAG) that specifies the reason why the charge balance equation could not be solved. The significance of the values of IFLAG are discussed in section 3.1 below.
6. LOOPSWITCH IS OUT OF RANGE

This is an error message that should never be printed if the program is functioning properly. LOOPSWITCH is a program variable whose value is determined by the XX portion of the DOLOOP XX control card and the program does not contain a statement capable of causing it to be out of range. This message was included as a check on the proper operation of the DOLOOP option.

### 2.3 ADDITIONAL INFORMATION

The program listing in section 4 of this report is copiously documented with comments to guide the user through the details of the program. The complete program, listed in section 4 , consists of a main program followed by a series of three subroutines and one function. The function TEST and the subroutine ZEROIN are used for finding the position of the Fermi level, and the subroutines MOB and SICI are used for performing the mobility computations. Notice that the mobility algorithm requires knowledge of many of the parameters calculated by the Fermi level locating routine; thus, it cannot be used without first finding the location of the Fermi level.

All of these routines have been written in FORTRAN IV for use on the Univac 1108 computer at the National Bureau of Standards. This is a 36-bit machine with 26-bit mantissa floating-point numbers. It may be necessary to use double precision to obtain a satisfactory accuracy on machines with significantly smaller word lengths. It may also be necessary to modify the alphanumeric format for data cards and the IF statements that test alphanumeric variables for machines that do not store six alphanumeric characters per word.

There are several places within the program where a zero denominator might occur during execution (e.g., when computing the Hall coefficient for a very small carrier density at low temperatures). The present program tests for this circumstance in all places where this has occurred in actual use. When this condition is encountered, a suitable flag is set, the division in question is circumvented, and the printing of all affected parameters is suppressed. In addition, all parameters with a zero value are omitted from the output listing so as not to clutter the output pages with multiple zero entries. This has been accomplished by preceding each WRITE statement with an appropriate IF statement that suppresses the printing of undesired output. Since this may slow down the printing speed or increase the cost of execution in some systems, the reader may wish to modify this portion of the program to achieve the same result with object-time format statements [6] computed during execution and stored in an array for use by the appropriate WRITE statement.

Copies of the main program are available on cards from the authors.

## 3. THEORY AND METHOD OF COMPUTATION

The computations of the position of the fermi level and carrier mobilities are key parts of this program. The various equations used in these computations are discussed below. Numbers cited in the following sections refer to statement numbers in the complete program given in section 4. If two numbers are given, the first refers to electrons or donor states, and the second to holes or acceptor states.

### 3.1 LOCATION OF THE FERMI LEVEL

For uniformly doped silicon in thermal equilibrium (as assumed herein), the summation of all negative charges must equal the summation of all positive charges (i.e., the material must be electrically neutral). The negative charges consist of electrons in the conduction band and any negatively charged impurity states (acceptors). The positive charges consist of holes in the valence band and any positively charged impurity states (donors). The Fermi level is located at just that point that makes the total net charge equal zero. The FORTRAN parameter TEST defined in statement 140 of the function TEST is a measure of how precisely the algorithm has located the position of the Fermi level to obtain charge neutrality.

$$
\begin{align*}
& \text { TEST }=(\text { Net negative charge })-(\text { Net positive charge) } \\
& \mathrm{TEST}=(\mathrm{CN}+\mathrm{DI} 3+D I 4+D I 5)-(C P+D I 1+D I 2) \tag{140}
\end{align*}
$$

where the symbols represent densities in reciprocal cubic centimeters as follows:

CN , electrons in the conduction band,
$C P$, holes in the valence band,
DI1, ionized donor species 1 ,

[^2]DI2, ionized donor species 2,
DI3, ionized acceptor species 3,
DI4, ionized acceptor species 4, and
DI5, ionized acceptor species 5.
The densities of electrons and holes in the conduction and valence bands, respectively, are computed using Blakemore's approximations to the FermiDirac integral [5]:

$$
\begin{equation*}
\mathrm{n}=\mathrm{N}[\exp (-n)+0.27]^{-1} \tag{8,26}
\end{equation*}
$$

for values of $\eta$ in the range from -80 to +1 ,

$$
\begin{equation*}
\mathrm{n}=0.752253 \mathrm{~N}\left(n^{2}+1.7\right)^{3 / 4} \tag{10,30}
\end{equation*}
$$

for values of $n$ greater than +1 , and

$$
\begin{equation*}
\mathrm{n}=0 \tag{2,20}
\end{equation*}
$$

for values of $n$ less than -80. In these equations, $n$ is the electron or hole density, $N$ is the density of states in the appropriate band, $n=q\left(E_{F}-\right.$ $\mathrm{E}_{\mathrm{g}}$ ) $/ \mathrm{kT}$ for electrons (4), and $-\mathrm{qE}_{\mathrm{F}} / \mathrm{kT}$ for holes (22), $\mathrm{E}_{\mathrm{F}}$ is the Fermi energy, in electron volts, $E_{g}$ is the width of the forbidden energy gap in electron volts (the zero of energy is assumed at the valence band edge), and $\mathrm{kT} / \mathrm{q}$ is the voltage equivalent of the temperature ( 353 of Main Program).

The density of states is given by

$$
\begin{aligned}
\mathrm{N} & =2\left(2 \pi \mathrm{k} \mathrm{~m} \mathrm{o}_{\mathrm{o}} / \mathrm{h}^{2}\right)^{3 / 2} \mathrm{~m}^{* 3 / 2} \mathrm{~T}^{3 / 2} \\
& =4.829 \times 10^{15} \mathrm{~m}^{\star 3 / 2} \mathrm{~T}^{3 / 2},
\end{aligned}
$$

(354,355) Main Program
where $\mathrm{m}^{*}$ is the effective mass of the appropriate carrier relative to the free electron mass, $m_{0}$. The relative electron effective mass, me, is given by [7] ${ }^{\dagger}$

$$
\begin{aligned}
\mathrm{m}_{\mathrm{e}}^{*} & =1.0627-1.61708 \times 10^{-4} \mathrm{~T}+6.83008 \times 10^{-6} \mathrm{~T} 2-3.32013 \times 10^{-8} \mathrm{~T}{ }^{3} \\
& +8.04032 \times 10^{-11} \mathrm{~T}^{4}-9.66067 \times 10^{-14} \mathrm{~T}^{5}+4.54649 \times 10^{-17} \mathrm{~T}^{6}
\end{aligned}
$$

(350) Main Program
and the relative hole effective mass, $\mathrm{m}_{\mathrm{h}}{ }^{*}$, is given by [7]
${ }^{\dagger}$ This and the following two equations have been carried to high order in kelvin temperature for purposes of computational accuracy, without regard to how high an order is really necessary to describe the measured data to within experimental accuracy.

$$
\begin{aligned}
\mathrm{m}_{\mathrm{h}}^{*} & =0.590525-5.23548 \times 10^{-4} \mathrm{~T}+1.85678 \times 10^{-5} \mathrm{~T}^{2}-9.67212 \times 10^{-8} \mathrm{~T}^{3} \\
& +2.30049 \times 10^{-10} \mathrm{~T}^{4}-2.596730 \times 10^{-13} \mathrm{~T}^{5}+1.11997 \times 10^{-16} \mathrm{~T}^{6}
\end{aligned}
$$

The temperature dependence of the forbidden energy gap of silicon is taken into account in accordance with a fit to the data of Macfarlane et al. [8]:

$$
\begin{aligned}
\mathrm{E}_{\mathrm{g}} & =1.15556+3.23741 \times 10^{-5} \mathrm{~T}-8.7011 \times 10^{-7} \mathrm{~T}^{2}+9.95401 \times 10^{-10} \mathrm{~T}^{3} \\
& -3.80977 \times 10^{-13} \mathrm{~T}^{4}
\end{aligned}
$$

(356) Main Program

The density of ionized impurities is computed from the following:

$$
\begin{equation*}
N_{i}=N_{t}[1+g \exp (\Delta)] \tag{40ff}
\end{equation*}
$$

where $\mathrm{N}_{\mathrm{t}}$ is the total density of the dopant impurity, g is the degeneracy factor, and $\Delta=q\left(E_{F}-E_{g}+E_{A}\right) / k T$ for donor states and $q\left(E_{A}-E_{F}\right) / k T$ for acceptor states, and $E_{A}$ is the value of the activation energy, relative to the appropriate band edge. This treatment of ionized impurity states is only valid for simple donor and acceptor states that have the following properties:

1. Each impurity state gives rise to only one electronic state. The present version of this program cannot handle the case of coupled multiple levels associated with a single impurity species unless the levels are widely separated and can be treated independently.
2. The donor levels are neutral when occupied by an electron and have a temperature-independent activation energy referenced to the bottom of the conduction band.
3. The acceptor levels are neutral when occupied by a hole and have a temperature-independent activation energy referenced to the top of the valence band.

These properties are appropriate for the column 3 and column 5 impurities in the periodic table (e.g., boron and phosphorus) and may, or may not, be appropriate for other impurities with larger activation energies or multiple energy levels. Impurity states satisfying these criteria are called dopant states in this report and are characterized by the following three parameters which are specified on the input data cards for each state:

1. the concentration of the dopant state per unit volume of silicon,
2. the limiting activation energy at low concentrations relative to the appropriate band edge, and
3. the degeneracy of the dopant state (an integer larger than unity).

The decrease in activation energy with increasing dopant density or increasing compensation is taken into account with the use of an equation based on
the work of Penin et al. [9] for phosphorus-doped silicon. Penin's expression gives zero activation energy at $3 \times 10^{18} \mathrm{~cm}^{-3}$ regardless of the initial activation energy, $\mathrm{E}_{\mathrm{AO}}$. Since deeper levels are expected to require greater densities to obtain zero activation energy [10], Penin's expression has been modified to retain the same decrease in activation energy, in eV, for a given increase in dopant density. To accomplish this, Penin's factor of $8 \times 0.045$, where 0.045 is the phosphorus activation energy, is fixed at 0.36. Thus, since $E_{A O}$ is greater for a deep level, the dopant density for zero activation energy is correspondingly greater.

The resulting equation for calculating the decrease in activation energy with dopant density and compensation is

$$
E_{A}=E_{A 0}-0.36\left(\frac{1}{2}+\frac{a^{*}}{r_{d}}\right) \exp \left(-r_{d} / a^{*}\right)-\alpha N_{2}^{1 / 3}
$$

(70 ff) Main Program
where $E_{A 0}$ is the activation energy for low densities of the dopant, $r_{\mathrm{d}}=$ $\left[3 /\left(4 \pi N_{1}\right)\right]^{1 / 3}$ is the average distance between the dominant dopant atoms of a given class (donor or acceptor), $a^{*}=21 \times 10^{-8} \mathrm{~cm}$ is the effective Bohr radius, $\alpha=3.6 \times 10^{-8} \mathrm{eV} \mathrm{cm}$, and $\mathrm{N}_{2}$ is the total density of compensating impurities of the other class (acceptor or donor). This equation is used in the computer program for all dopant states, but its applicability to deep levels has not been verified.

Since the reduction in activation energy with increasing donor density is due in large part to the lowering of the bottom of the conduction band, the total donor density is used in the calculation of the reduction for each donor state. Likewise, when more than one acceptor state is present, the total acceptor state density is used to calculate the reduction in activation energy of each acceptor state. However, when two or more donors (or acceptors) are present, each in significant quantity, this approach probably overestimates the reductions in activation energy of each acceptor state.

The computation of the reduction in activation energy is not included as part of the routine for finding the Fermi level, but has been included in the Main Program as part of the initialization procedure. The routine for finding the Fermi level position assumes that the values of activation energy previously placed in COMMON are the correct values. The complete program outputs both the limiting value of activation energy initially inputted and the calculated lowered value of activation energy (see sec. 5).

The correct position of the Fermi level is found by the subroutine ZEROIN [11-13] which searches for a zero of the parameter TEST. ZEROIN is listed as part of the complete program in section 4. The subroutine is well documented with descriptive comments before the code and explanations of all significant steps as they occur in the body of the code. The subroutine looks for a zero between the variables EF and EFG which are given initial values of 0.0 and 1.2 eV , respectively, by the calling program. In searching for the root, ZEROIN uses the secant rule unless tests indicate that bisection would be advantageous. The interval between EF and EFG is narrowed until the stopping criterion is satisfied. The stoppirg criterion is

$$
\left|\frac{E F-E F G}{2}\right| \leq R E \times E F+A E
$$

where $R E$ is the maximum allowable relative error and $A E$ is the maximum allowable absolute error in eV . In the calling program these are both assigned the value $1 \times 10^{-6}$ so that they have equal weight in the stopping criterion when $E F=1.0 \mathrm{eV}$. Initially, the subroutine compares $R E$ with the roundoff error of the machine, ER, specified in a DATA statement, which can be easily changed to correspond to the user's computer, and selects the larger of the two for the stopping criterion.

At the conclusion of the computations, EF is the better approximation to the zero of TEST as the subroutine, by interchange if necessary, makes $|\operatorname{TEST}(E F)|<|\operatorname{TEST}(E F G)|$. Before the return to the main program, the parameter IFLAG is set to indicate the status of the results. The normal case with the root located within the stopping criterion is denoted by IFLAG $=1$. A possible, but unlikely, result is $\operatorname{TEST}(E F)=0$ without the stopping criterion being met (current value of EFG not close enough to EF). For this situation IFLAG $=2$. If the stopping criterion is met, but $\mid$ TEST (EF) |is larger than the absolute value of TEST evaluated with either initial argument, IFLAG $=3$. If the stopping criterion is satisfied, but TEST(EF) x TEST (EFG) > 0, there is apparently no root in the interval and IFLAG $=4$. ZEROIN permits up to 500 evaluations of TEST before terminating and setting IFLAG $=5$. If upon return to the main program IFLAG is not 1 or 2 , its value is printed for diagnostic purposes. The program then proceeds to the next temperature. For a successful evaluation (IFLAG $=1$ or 2 ), the residual value of TEST, called TESTF, is printed in the DOUBLE ON output listing.

### 3.2 COMPUTATION OF CARRIER MOBILITIES AND RELATED PARAMETERS

The scattering mechanisms which are included in the calculation of the carrier mobility are lattice, ionized impurity, neutral impurity, and electronelectron (or hole-hole) interactions. The mobility calculations are summarized in the tables which follow. In table 1 , the symbols used in the mobility formulas are defined and the corresponding computer program name is given. Table 2 gives the mathematical formulas for calculating electron mobility along with the statement number of the corresponding expression in the computer program. Table 3 gives this information for the calculation of hole mobility.

The temperature dependence of the electron mobility due to lattice scattering is taken from the work of Norton et $a l$. [14], and the magnitude is based on the results at 300 K of Thurber et $\alpha$. [15]. The temperature dependence of this mobility changes slope at about 110 K , and this is the reason for the different equations in table 2. For holes, the lattice mobility for temperatures below 72 K is from Braggins [16], whereas at higher temperatures the results of Ludwig and Watters [17] are used.

The ionized impurity scattering mobility is calculated by the Brooks-Herring [18,19] expression, with the modifications discussed by Li and Thurber [20] and Li [21]. For p-type material, individual mobilities are computed for each band, and then the total mobility is found by weighting the mobility in each band by the hole density in that band. The effect of carrier-carrier

Table 1. Symbols Used in Mobility Formulas.

| Mathematical Symbol | Program Name | Definition* |
| :---: | :---: | :---: |
| $N_{D}$ | SUMTD | Total donor density ( $\mathrm{cm}^{-3}$ ) |
| $\mathrm{N}_{\text {A }}$ | SUMTA | Total acceptor density ( $\mathrm{cm}^{-3}$ ) |
| ${ }^{\mu}$ | ULN | Lattice mobility for electrons ( $\mathrm{cm}^{2} / \mathrm{V} \cdot \mathrm{s}$ ) |
|  | ULP | Lattice mobility for holes ( $\mathrm{cm}^{2} / \mathrm{V} \cdot \mathrm{s}$ ) |
| ${ }^{\mu}$ I | UIN | Ionized impurity mobility for electrons ( $\mathrm{cm}^{2} / \mathrm{V} \cdot \mathrm{s}$ ) |
|  | UIP | Ionized impurity mobility for holes ( $\mathrm{cm}^{2} / \mathrm{V} \cdot \mathrm{s}$ ) |
| $\gamma$ | GAMMA | Factor giving effect of carrier-carrier scattering on ionized impurity mobility |
| $\mathrm{N}_{\text {I }}$ | CION | Density of ionized impurities ( $\mathrm{cm}^{-3}$ ) |
| $G(b)$ | GN | Log term in Brooks-Herring ionized impurity mobility formula for electrons |
|  | GP | Log term in Brooks-Herring ionized impurity mobility formula for holes |
| $\mathrm{N}_{\mathrm{D}}{ }^{+}$ | SUMID | Total ionized donor density ( $\mathrm{cm}^{-3}$ ) |
| $\mathrm{N}_{\mathrm{A}}{ }^{+}$ | SUMIA | Total ionized acceptor density ( $\mathrm{cm}^{-3}$ ) |
| $n^{\prime}$ | CNSTAR | Effective electron screening density ( $\mathrm{cm}^{-3}$ ) |
| $p^{\prime}$ | CPSTAR | Effective hole screening density ( $\mathrm{cm}^{-3}$ ) |
| $4 \pi \kappa \varepsilon_{0}$ | DIEL | $4 \pi$ times relative dielectric constant times permittivity of free space |
| k |  | Boltzmann constant |
| h |  | Planck constant ( $\dagger=h / 2 \pi$ ) |
| 9 |  | Electronic charge |
| $\mathrm{m}_{0}$ |  | Free electron mass |
| $\mathrm{m}_{\ell}{ }^{\text {* }}$ |  | Longitudinal effective mass (in units of $\mathrm{m}_{0}$ ) |
| $\pi_{d}{ }^{*}$ |  | Density-of-states effective mass (in units of $m_{0}$ ) |
| $\mathrm{m}_{\mathrm{c}}{ }^{\text {* }}$ |  | Conductivity effective mass (in units of $m_{0}$ ) |
| ${ }^{\mu} \mathrm{N}$ | UNIS | Neutral impurity scattering mobility ( $\mathrm{cm}^{2} / \mathrm{V} \cdot \mathrm{s}$ ) |
| $\mathrm{N}_{\mathrm{N}}$ | CNUT | Density of neutral impurities ( $\mathrm{cm}^{-3}$ ) |
| n | CN | Electron density ( $\mathrm{cm}^{-3}$ ) |
| p | CP | Hole density ( $\mathrm{cm}^{-3}$ ) |

[^3]Table 2. Formulas for Calculating Electron Mobility.

| Scattering $\quad$ Formula Mechanism | Statement Number |
| :---: | :---: |
| $\begin{array}{lll} \hline \begin{array}{l} \text { Lattice }+ \\ \text { electron-electron } \end{array} & N_{D}<3 \times 10^{17} \mathrm{~cm}^{-3} \\ & T \leq 108 \mathrm{~K} & \mu_{\mathrm{L}}=1.89 \times 10^{7} \mathrm{~T}^{-1.52}\left[1-0.08 \mathrm{~N}_{\mathrm{D}} /\left(2 \times 10^{17}\right)\right] \\ & \mathrm{T}>108 \mathrm{~K} & \mu_{\mathrm{L}}=7.98 \times 10^{8} \mathrm{~T}^{-2.32}\left[1-0.08 \mathrm{~N}_{\mathrm{D}} /\left(2 \times 10^{17}\right)\right] \\ & & N_{D} \geq 3 \times 10^{17} \mathrm{~cm}^{-3} \\ & \mathrm{~T} \leq 108 \mathrm{~K} & \mu_{\mathrm{L}}=1.89 \times 10^{7} \mathrm{~T}-1.52(0.884) \\ & \mathrm{T}>108 \mathrm{~K} & \mu_{\mathrm{L}}=7.98 \times 10^{8} \mathrm{~T}^{-2.32}(0.884) \end{array}$ | $\begin{array}{r} 8 \\ 10 \\ 22 \\ 30 \end{array}$ |
| $\begin{array}{ll} \begin{array}{l} \text { Ionized impurity } \\ \text { electron-electron } \end{array} & \mu_{I}=\gamma \times 7.3 \times 10^{17} T^{1} \cdot 5 / N_{I} G(b) \\ & \gamma=\frac{N_{D}{ }^{+}}{n^{\prime}}\left[1-\exp \left(-n^{\prime} / N_{D}{ }^{+}\right)\right] \\ n^{\prime}=n+p+N_{D}^{+}\left(1-N_{D^{+}} / N_{D}\right) \\ G(b)=\ln (b+1)-b /(b+1) \\ & b=\frac{24_{k} \varepsilon_{0} m_{l}^{*}(k T)^{2}}{q^{2} \hbar^{2} n^{\prime}} \times 10^{-6} \end{array}$ | $\begin{aligned} & 90 \\ & 86 \\ & 42 \\ & 80 \\ & 52 \end{aligned}$ |
| $\begin{array}{ll} \text { Combined lattice } & \mu_{L I}=\mu_{L} f(X) \\ \text { and ionized im- } \\ \text { purity } & f(X)=1+X^{2}\left[\operatorname{CiX} \cos X+\sin X\left(\operatorname{Six}-\frac{\pi}{2}\right)\right] \\ & X^{2}=6 \mu_{L} / \mu_{I} \end{array}$ | $\begin{array}{r} 104 \\ 104 \\ 98 \end{array}$ |
| Neutral impurity $\begin{aligned} & \mu_{N}=0.32 \mu_{E}\left[\frac{2}{3}\left(\frac{k T}{E_{N}}\right)^{1 / 2}+\frac{1}{3}\left(\frac{E_{N}}{k T}\right)^{1 / 2}\right] \\ & E_{N}=\frac{1.136 \times 10^{-19} m_{d}^{\star}}{\kappa^{2} m_{0}} \\ & \mu_{E}=\frac{2 \pi^{3} q^{3} m_{d}^{\star}}{5 N_{N} 4 \pi \kappa \varepsilon_{0} h^{3}} \times 10^{-2} \end{aligned}$ | 114 112 110 |
| $\begin{aligned} & \text { Total electron } \\ & \text { mobility }\end{aligned} \quad \mu=\left(1 / \mu_{\text {LI }}+1 / \mu_{N}\right)^{-1}$ | 116 |

Table 3. Formulas for Calculating Hole Mobility.

\begin{tabular}{|c|c|c|}
\hline Scattering Mechanism \& Formula \& Statement Number* \\
\hline Lattice + hole-hole \& \[
\begin{aligned}
\& N_{A}<3 \times 10^{17} \mathrm{~cm}^{-3} \\
T<72 \mathrm{~K} \quad \mu_{\mathrm{L}}= \& 1.6 \times 10^{7} \mathrm{~T}-1.54\left[1-0.08 \mathrm{~N}_{A} /\left(2 \times 10^{17}\right)\right] \\
\mathrm{T} \geq 72 \mathrm{~K} \quad \mu_{\mathrm{L}}= \& 2.3 \times 10^{9} \mathrm{~T}^{-2.7}\left[1-0.08 \mathrm{~N}_{A} /\left(2 \times 10^{17}\right)\right] \\
\& N_{A} \geq 3 \times 10^{17} \mathrm{~cm}^{-3} \\
\mathrm{~T}<72 \mathrm{~K} \quad \mu_{\mathrm{L}}= \& 1.6 \times 10^{7} \mathrm{~T}^{-1.54}(0.884) \\
\mathrm{T} \geq 72 \mathrm{~K} \quad \mu_{\mathrm{L}}= \& 2.3 \times 10^{9} \mathrm{~T}-2.7(0.884)
\end{aligned}
\] \& \begin{tabular}{l}
118 \\
120 \\
132 \\
140
\end{tabular} \\
\hline \begin{tabular}{l}
Ionized impurity \\
+ hole-hole
\end{tabular} \& \begin{tabular}{l}
\[
\begin{aligned}
\& \mu_{I}=\frac{\gamma\left[\mu_{I 7}+\mu_{I 2}\left(m_{d 2}^{*} / m_{d 7}^{*}\right)^{1.5}+\mu_{I 3}\left(m_{d 3}^{*} / m_{d 7}^{*}\right)^{1.5} \exp (-0.044 / k T)\right]}{\left[1+\left(m_{d 3}^{*} / m_{d 7}^{*}\right)^{1.5}+\left(m_{d 3}^{*} / m_{d 7}^{*}\right)^{1.5} \exp (-0.044 / k T)\right]} \\
\& \gamma=\frac{N_{A}^{+}}{p^{\prime}}\left[1-\exp \left(-p^{\prime} / N_{A}^{+}\right)\right] \\
\& p^{\prime}=p+n+N_{A}^{+}\left(1-N_{A}^{+} / N_{A}\right)
\end{aligned}
\] \\
for \(i=1,2,3\)
\[
\begin{aligned}
\& \mu_{I i}=\frac{2^{3.5}\left(4 \pi k \varepsilon_{0}\right)^{2} m_{d i}^{*}{ }^{0.5}(k T)^{1.5}}{\pi^{1.5} q^{3} m_{c i}^{*} N_{I} G\left(b_{i}\right)} \times 10^{-2} \\
\& G\left(b_{i}\right)=\ln \left(b_{i}+1\right)-b_{i} /\left(b_{i}+1\right) \\
\& b_{i}=\frac{24 k \varepsilon_{0} m_{d i}^{*}(k T)^{2}}{q^{2} \hbar^{2} p^{1}} \times 10^{-6}
\end{aligned}
\]
\end{tabular} \& 196
198
152

192
190
162 <br>

\hline Combined lattice and ionized impurity \& $$
\begin{aligned}
& \mu_{L I}=\mu_{L} f(X) \\
& f(X)=1+X^{2}\left[\operatorname{Ci} X \cos X+\sin X\left(\operatorname{six} X-\frac{\pi}{2}\right)\right] \\
& X^{2}=6 \mu_{L} / \mu_{I}
\end{aligned}
$$ \& \[

$$
\begin{aligned}
& 214 \\
& 214 \\
& 208
\end{aligned}
$$
\] <br>

\hline
\end{tabular}

| Neutral impurity |  | 224 222 221 220 |
| :---: | :---: | :---: |
| Total hole mobility | $\mu=\left(1 / \mu_{L I}+1 / \mu_{N}\right)^{-1}$ | 226 |

* These statement numbers refer to subroutine MOB.
scattering in reducing the lattice and ionized impurity mobilities is taken into account following the work of Li and Thurber [20]. The mobility due to both lattice and ionized impurity scattering is combined according to the mixed-scattering formula of Debye and Conwell [22] involving sine and cosine integrals.

The expressions used to calculate the carrier mobilities contain the dielectric constant of silicon as a parameter. The value of 11.7 for the relative dielectric constant of silicon at 300 K was taken from Dunlap and Watters [23]. The temperature variation was calculated from the index of refraction data of Cardona et al. [24], assuming that the index of refraction is the square of the relatjve dielectric constant. The resulting expression for the program parameter DIEL evaluated in subroutine MOB statement No. 2 is:

```
DIEL = 4 (absolute dielectric constant) and
DIEL = (1.2711 x 10-9) exp(7.8 x 10-5}\textrm{T})\mathrm{ farads per meter.
```

The neutral impurity scattering mobility is calculated from the Erginsoy equation [25], with the modification proposed by Sclar [26]. The net mobility is found by combining reciprocally the neutral impurity mobility with the result for the combined lattice and ionized impurity mobility.

Both electron and hole mobilities are calculated, even though usually only one carrier is important. An effective conductivity mobility is calculated by summing the electron and hole mobilities weighted by the density of each carrier. The effective conductivity mobility computed this way is the same as the majority carrier conductivity mobility in extrinsic specimens. In intrinsic specimens, it corresponds to a hypothetical mobility for the total carrier density (i.e., electron plus hole density). The effective conductivity mobility is the only value of mobility listed in the no-option output format. Additional mobility values are available in the DOUBLE ON output format. The expressions for calculating the conductivity, resistivity, and Hall coefficient include appropriately weighted contributions from both charge carriers.

PROGRAM CAN HANDLE 2 DONOR LEVELS AND 3 ACCEPTOR LEVELS

VARIABLE NAMES

| LEVEL | NAME | DENSITY | ENERGY | DEGEN. | ION. CONC. |
| :--- | :--- | :--- | :--- | :--- | :--- |
|  |  |  |  |  |  |
| DONOR 1 | NAME1 | DN1 | ENIN1 | DG1 | DI1 |
| DONOR 2 | NAME2 | DN2 | ENIN2 | DG2 | DI2 |
| ACCEPTOR 1 | NAME3 | DN3 | ENIN3 | DG3 | DI3 |
| ACCEPTOR 2 NAME4 | DN4 | ENIN4 | DG4 | DI4 |  |
| ACCEPTOR 3 NAME5 | DN5 | ENIN5 | DG5 | DI5 |  |

STATEMENT NUMBERS ENDING IN ZERO ARE PART OF THE PROGRAM LOGIC OTHER NUMBERS WERE ADDED FOR IDENTIFICATION PURPOSES A MODIFIED MKS SYSTEM OF UNITS IS USED WITH CM REPLACING METERS

T = THE TEMPERATURE IN KELVIN
$E G=$ THE ENERGY GAP OF SILICON IN ELECTRON VOLTS
EXCITON ENERGY OF 0.01 EV IS NOT INCLUDED IN EG
$E F=F E R M I$ LEVEL IN EV (DETERMINED IN PROGRAM BY TRIAL AND ERROR)
EF IS TAKEN TO BE ZERO AT THE VALENCE BAND EDGE
$C N=$ THE CONCENTRATION OF ELECTRONS IN THE CONDUCTION BAND IN CM-3
$C P=$ THE CONCENTRATION OF HOLES IN THE VALENCE BAND IN CM-3
MOB = MOBILITY ON THE OUTPUT PAGES, BUT NOT IN THE PROGRAM:
IN THE PROGRAM, THE FOLLOWING NOTATION IS USED: UDN $=$ THE ELECTRON MOBILITY IN CM**2/(VOLT-SEC) UDP $=$ THE HOLE MOBILITY IN CM**2/(VOLT-SEC) UD = THE CONDUCTIVITY MOBILITY IN CM**2/(VOLT-SEC)
RH $=$ THE HALL COEFFICIENT IN CM**3/COULOMB
SIGMA $=$ THE CONDUCTIVITY IN MHO/CM
RHO = THE RESISTIVITY IN OHM-CM
ON THE OUTPUT PAGE THE FOLLOWING NOTATION HAS BEEN USED:
D1 ION = THE DENSITY OF IONIZED DONOR 1 IN CM-3
D2 ION = THE DENSITY OF IONIZED DONOR 2 IN CM-3
A1 ION = THE DENSITY OF IONIZED ACCEPTOR 1 IN CM-3
A2 ION = THE DENSITY OF IONIZED ACCEPTOR 2 IN CM-3
A3 ION = THE DENSITY OF IONIZED ACCEPTOR 3 IN CM-3
FNC AND FNV ARE THE DENSITY OF STATES IN THE CONDUCTION AND VALENCE BANDS RESPECTIVELY IN CM-3

INPUT DATA CARDS:
ORDER OF CARDS IS THE SAME AS IN THE TABLE ABOVE ORDER OF DATA ON CARD = NAME, DENSITY, ENERGY, DEGEN. TO ELIMINATE A LEVEL FROM THE PROGRAM, NAME IT 'DUMMY' THE LAST DATA CARD SHOULD READ SIMPLY 'STOP'

THE FIRST DATA CARD OF ANY SET CAN BE USED TO CONTROL THE PROGRAM SEE THE LIST OF IF STATEMENTS FOLLOWING STATEMENT 10 FOR SUCH USE 'DOUBLE ON' TURNS ON 2 OUTPUT DATA LINES AT EACH TEMP.

C PERFORM THE NECESSARY DOLOOP INSTRUCTIONS
DO 720 NRUN=1,NDIT,1
IF (NRUN.EQ.1.) GO TO 50
IF (LOOPSW.EQ.1.) DN1=DN1+DELDEN
IF (LOOPSW.EQ.2.) DN2=DN2+DELDEN
IF (LOOPSW.EQ.3.) DN3=DN3+DELDEN
IF (LOOPSW.EQ.4.) DN4=DN4+DELDEN
IF (LOOPSW.EQ.5.) DN5=DN5+DELDEN
IF (LOOPSW.GT.5.) GO TO 30
GO TO 50
PRINT 40
FORMAT ( $1 \mathrm{HO}, 26 \mathrm{HLOOPSWITCH}$ IS OUT OF RANGE)
GO TO 10
'DOUBLE OFF' RESTORES SINGLE OUTPUT LINE FORMAT CHANGE WITH DOPING LEVEL
'DOLOOP XX' (WHERE XX = D1 - A3) PRODUCES MULTIPLE RUNS

EXTERNAL TEST
DIMENSION NAME1 (2), NAME2 (2), NAME3 (2) ,NAME4 (2), NAME5 (2)
COMMON NAME1,NAME2,NAME3,NAME4,NAME5
COMMON DN1,DN2,DN3,DN4,DN5,SUMTD,SUMTA
COMMON DI1,DI2,DI3,DI4,DI5
COMMON EN1,EN2,EN3,EN4,EN5
COMMON DG1,DG2,DG3,DG4,DG5
COMMON T, CN, CP, EG, EFME,EFMH,FNC,FNV,CAYT, TPOWR, Q, ALPHA,BETA
COMMON UD, UDN, ULN, UDP, ULP, SIGMA, RHO, RH
COMMON OUT8,OUT11,ISTAT
$Q=1.6022 \mathrm{E}-19$
INITIALIZE THE SETTINGS OF THE OPTION SWITCHES LOOPSW=0.
DOUBSW $=6 \mathrm{HOFF}$
READ THE D1 DATA (OR CONTROL) CARD
0 READ 20, NAME1,DN1,ENIN1,DG1
IF (NAME1 (1).EQ.6HDOUBLE) GO TO 730
IF (NAME1 (1).EQ.6HCONSTA) GO TO 50
IF (NAME1 (1).EQ. 6HDOLOOP) GO TO 740
IF (NAME1 (1).EQ.6HSTOP ) GO TO 760
READ THE REMAINING FOUR DATA CARDS
READ 20, NAME2,DN2,ENIN2,DG2
READ 20, NAME3,DN3,ENIN3,DG3
READ 20, NAME4,DN4,ENIN4,DG4
READ 20, NAME5,DN5, ENIN5,DG5
FORMAT (2A6,E10.4,2F10.4)
IF (LOOPSW.EQ.O.) GO TO 50

RUNNO=1. DURING FIRST RUN, THEN 2. UP TO 77 KELVIN, THEN 3. TO ROOM TEMPERATURE, THEN 4. ABOVE ROOM TEMPERATURE RUNNO $=1$.
'CONSTANTS' GENERATES A PAGE OF THE PARAMETERS THAT DO NOT CARD FORMAT $=$ DOLOOP XX, INC. DENSITY, NO. OF RUNS 'STOP' IS USED TO TERMINATE THE SESSION WITH THE COMPUTER

| C | CALULATE REDUCTION IN ACTIVATION ENERGIES |
| :---: | :---: |
| C | EQUATION OF PENIN ET AL. FOR PHOSPHORUS-DOPED SILICON IS |
| C | GENERALIZED FOR USE WITH OTHER ACTIVATION ENERGIES |
| C | SEE PAPER IN SOVIET PHYS.-SOLID STATE 7, 2580 (1966) |
|  | SUMTD $=$ DN1+DN2 |
| c | GUARD AGAINST ZERO DIVISOR IN CALCULATION OF RDDIF (SUMTD.LE.O.) RDD=1.E20 |
|  |  |
|  | IF (SUMTD.LE.O.) GO TO 60 |
|  | RDD $=1 . \mathrm{E8*}$ (3.1(4.*3.1416*SUMTD ) ) **0.3333 |
| 60 | SUMTA $=$ DN3+DN4+DN5 |
| c | GUARD AGAINST ZERO DIVISOR IN CALCULATION OF RDA |
|  | If (SUMTA.LE.O.) RDA=1.E20 |
|  | IF (SUMTA.LE.O.) GO TO 70 |
|  | RDA $=1 . \mathrm{E}$ ** (3.1(4.*3.1416*SUMTA) ) **0.3333 |
| 70 | EN1=ENIN1 |
| C | FOLLOWING STATEMENT COMPUTES THE REDUCTION IN ACTIVATION ENERGY |
| C | OMIT THIS STATEMENT IF FIXED ENERGY LEVEL ENIN1 IS DESIRED |
| C | SAME COMMENTS APPLY TO OTHER DOPANT STATES |
|  | EN1=ENIN1-0.36* (0.5+21./RDD)*EXP (-RDD/21.)-3.6E-8*SUMTA**0.3333 |
| C | IF ANY ACTIVATION ENERGY IS NEGATIVE, SET IT EQUAL TO ZERO |
| 80 | EN1 $=0.0$ |
| 90 | EN2=ENIN2 |
|  | $\begin{aligned} & \text { EN2 }=\text { ENIN2-0.36*(0.5+21./RDD }) * E X P(-R D D / 21 .)-3.6 E-8 * S U M T A * * 0.3333 \\ & \text { IF }(E N 2-0.0) 100,110,110 \end{aligned}$ |
| 100 | EN2=0.0 |
| 110 | EN3=ENIN3 |
|  | ```EN3=ENIN3-0.36*(0.5+21./RDA)*EXP(-RDA/21.)-3.6E-8*SUMTD**0.3333 IF (EN3-0.0) 120,130,130``` |
|  |  |
| 120 | EN3 $=0.0$ |
| 130 | EN4=ENIN4 |
|  | EN4 $=$ ENIN4-0.36* (0.5+21./RDA) *EXP (-RDA/21.)-3.6E-8*SUMTD**0.3333 |
|  | IF (EN4-0.0) 140,150,150 |
| 140 | EN4 $=0.0$ |
| 150 | EN5=ENIN5 |
|  | ```EN5=ENIN5-0.36*(0.5+21./RDA)*EXP (-RDA/21.)-3.6E-8*SUMTD**0.3333 IF (EN5-0.0) 160,170,170``` |
| 160 | ENS $=0.0$ |
| C | THE FIRST TEMPERATURE WILL BE 4.2 KELVIN |
| 170 | $\mathrm{T}=4.2$ |
| C | T WILL BE INCREMENTED IN EQUAL 1000/T INTERVALS |
| C |  |
| C | SET UP THE OUTPUT PAGE |
|  | WRITE $(6,180)$ |
| 180 | FORMAT ( $1 \mathrm{H} 1,32 \mathrm{HELECTRICAL}$ PROPERTIES OF SILICON) |
|  | IF (NAME1 (1).EQ.6HCONSTA) GO TO 320 |
| C | READ-OUT ALL PERTINENT INPUT DATA |
|  | WRITE $(6,190)$ |
| 190 | FORMAT ( $1 \mathrm{HO}, 26 \mathrm{HDOPANT}$ STATES FOR THIS RUN) |
|  | WRITE $(6,200)$ |
| 200 | FORMAT (1H0,77H DOPANT DENSITY ENERGY(INPUT) |
|  | 2NERGY(CALC.) DEGENERACY) |



```
    IF (NAME1 (1).EQ.6HCONSTA) GO TO 530
    EF=0.0
    EFG=1.2
    RE=1.OE-6
    AE=1.OE-6
    IFLAG=0
    C
    C
    C
    3 6 0
    3 7 0
    3 8 0
    390
    4 0 0 ~ F O R M A T ~ ( 2 O X , 7 2 H B O R N ~ A P P R O X I M A T I O N ~ F O R ~ I O N I Z E D ~ S C A T T E R I N G ~ N O T ~ V A L I D ~
    2 FOR MAJORITY CARRIER)
C
C OUTPUT THE RESULTS AND SET UP THE NEXT RUN
    WRITE (6,410) T,RTEMP,EF
    410 FORMAT (F11.4,2X,F9.4,F11.6)
    IF (CN.NE.O.) WRITE (6,420) CN
    IF (CP.NE.O.) WRITE (6,430) CP
    IF (UD.NE.O.) WRITE (6,440) UD
    IF (RH.NE.9.999999E19.AND.RH.NE.O.) WRITE (6,450) RH
    IF (RH.NE.9.999999E19.AND.RHO.NE.O.) WRITE (6,460) RHO
    IF (DI1.NE.O.) WRITE (6,470) DI1
    IF (DI2.NE.O.) WRITE (6,480) DI2
    IF (DI3.NE.O.) WRITE (6,490) DI3
    IF (DI4.NE.O.) WRITE (6,500) DI4
    420 FORMAT (1H+,33X,1PE11.3)
    430 FORMAT (1H+,44X,1PE11.3)
    440 FORMAT (1H+,55X,1PE11.3)
    450 FORMAT (1H+,66X,1PE11.3)
    460 FORMAT (1H+,77X,1PE11.3)
    470 FORMAT (1H+,88X,1PE11.3)
    480 FORMAT (1H+,99X,1PE11.3)
    490 FORMAT (1H+,110X,1PE11.3)
    5 0 0 ~ F O R M A T ~ ( 1 H + , 1 2 1 X , 1 P E 1 0 . 3 )
    IF (DOUBSW.NE.6HON ) GO TO 590
    OUT3=EG-EF
    TESTF=TEST(EF)
    WRITE (6,510) EG,TESTF,CAYT,OUT3
    5 1 0
    FORMAT (F11.6,1PE11.3,1PE11.4,2X,F9.6)
    IF (DI5.NE.O.) WRITE (6,430) DI5
```

```
    IF (RH.NE.9.999999E19.AND.SIGMA.NE.O.) WRITE (6,440) SIGMA
    IF (ULN.NE.O.) WRITE (6,450) ULN
    IF (OUT8.NE.O.) WRITE (6,460) OUT8
    IF (UDN.NE.O.) WRITE (6,470) UDN
    IF (ULP.NE.O.) WRITE (6,480) ULP
    IF (OUT11.NE.O.) WRITE (6,490) OUT11
    IF (UDP.NE.0.) WRITE (6,500) UDP
    WRITE (6,520)
    FORMAT (1HO)
    GO TO 590
C OUTPUT INSTRUCTIONS FOR THE 'CONSTANTS' OPTION
530 RDIEL=11.4294*EXP (7.8E-5*T)
    IF (T.GE.108.) GO TO 540
    ULN=1.89E7*T**(-1.52)
    GO TO 550
540 ULN=7.98E8*T**(-2.32)
550 IF (T.GE.72.) GO TO 560
    ULP=1.6E7*T**(-1.54)
    GO TO 570
    ULP=2.3E9*T**(-2.7)
5 7 0 \text { WRITE (6,580) T,RTEMP,CAYT,EG,RDIEL,ULN,ULP,TPOWR,EFME,EFMH,FNC,FN}
    2V
580 FORMAT (OP2F11.4,1PE11.4,2X,OPF9.4,F11.4,1P7E11.3)
C SET UP NEXT TEMPERATURE
C THE MAXIMUM TEMPERATURE OF INTEREST IS 500 DEGREES KELVIN
590 IF (T-500.) 600,710,710
600 IF (RUNNO-2.) 610,620,630
610 RUNNO=2.
C SECOND TIME AROUND, THE TEMPERATURE WILL BE 2O DEGREES KELVIN
    T=20.
    RTEMP=1000. / T
    GO TO 350
C AFTER THE SECOND TIME AROUND, 1000./T IS DECREMENTED BY 2.
620 RTEMP=RTEMP-2.
    T=1000./RTEMP
C AN EVALUATION AT LIQUID NITROGEN TEMPERATURE IS DESIRED
    IF (T.GE.77.) GO TO 640
    GO TO 350
6 3 0 ~ I F ~ ( T . E Q . 7 7 . ) ~ G O ~ T O ~ 6 5 0 ~
C AN EVALUATION AT ROOM TEMPERATURE (300 KELVIN) IS DESIRED
    IF (RUNNO.EQ.4.) GO TO 680
    IF (T.EQ.300.) GO TO 670
C FROM 77 KELVIN TO ROOM TEMPERATURE, 1000/T IS DECREMENTED BY 1.
    RTEMP=RTEMP-1.
    T=1000./RTEMP
    IF (T.GT.300.) GO TO 660
    GO TO 350
640 T=77.
    RTEMP=1000. / 
    RUNNO=3.
    GO TO 350
        RTEMP=12.
        T=1000. / RTEMP
```

```
    GO TO 350
6 6 0
    T=300.
    RTEMP=1000. / T
    GO TO 350
670 RTEMP=3.
    T=1000./RTEMP
    RUNNO=4.
    GO TO 350
C ABOVE ROOM TEMPERATURE 1000./T IS DECREMENTED BY 0.5
680 RTEMP=RTEMP-0.5
    T=1000. / RTEMP
    GO TO 350
    WRITE (6,700) IFLAG
700 FORMAT (1HO,51HCHARGE BALANCE EQUATION COULD NOT BE SOLVED, IFLAG=
    2,I1)
    GO TO 590
710 IF (DOUBSW.NE.6HON ) GO TO 720
C INITIALIZE CERTAIN VARIABLES FOR NEXT RUN
    ULN=0.
    OUT8=0.
    UDN=0.
    ULP=0.
    OUT11=0.
    UDP=0.
720 CONTINUE
    IF (NAME1(1).EQ.6HCONSTA) GO TO 10
    LOOPSW=0.
    HEADSW=6HOFF
    GO TO 10
C ROUTINE TO SET-UP OR CANCEL DOUBLE OUTPUT LINE FORMAT
C DOUBSW IS A SWITCH USED TO CONTROL THE OUTPUT FORMAT
730 DOUBSW=6HON
    IF (NAME1 (2).EQ.6HON ) GO TO 10
    IF (NAME1(2).EQ.6H ON ) GO TO 10
C DEFAULT VALUE IS TAKEN TO MEAN 'DOUBLE OFF'
    DOUBSW=6HOFF
    GO TO 10
C ROUTINE TO SET-UP DOLOOP OPTION
740 DELDEN=DN1
    NDIT=ENIN1
    IF (NAME1 (2).EQ.6H D1 ) LOOPSW=1.
    IF (NAME1 (2).EQ.6H D2 ) LOOPSW=2.
    IF (NAME1 (2).EQ.6H A1 ) LOOPSW=3.
    IF (NAME1 (2).EQ.6H A2 ) LOOPSW=4.
    IF (NAME1 (2).EQ.6H A3 ) LOOPSW=5.
    IF (LOOPSW.EQ.O.) WRITE (6,750)
750 F.ORMAT (1HO,34HINVALID ARGUMENT OF DOLOOP COMMAND)
    GO TO 10
760 STOP
    END
```

        THIS EXTERNAL FUNCTION DEFINES THE PARAMETER 'TEST'.
    C SUBROUTINE ZEROIN LOCATES THE VALUE OF EF WHICH MINIMIZES 'TEST'.
DIMENSION NAME1 (2), NAME2 (2), NAME3 (2), NAME4 (2), NAME5 (2)
COMMON NAME1, NAME2, NAME3,NAME4,NAME5
COMMON DN1,DN2,DN3,DN4,DN5,SUMTD,SUMTA
COMMON DI1,DI2,DI3,DI4,DI5
COMMON EN1,EN2,EN3,EN4,EN5
COMMON DG1,DG2,DG3,DG4,DG5
COMMON T, CN, CP, EG, EFME,EFMH,FNC, FNV, CAYT, TPOWR, Q, ALPHA, BETA
COMMON UD,UDN,ULN,UDP,ULP,SIGMA, RHO,RH
COMMON OUT8,OUT11,ISTAT
C
C COMPUTATION OF CN
$2 \quad C N=0$.
$4 \quad A L P H A=(E F-E G) / C A Y T$
IF (ALPHA.GT.1.) GO TO 10
IF (ALPHA.LE.-80.) GO TO 20
C THE FOLLOWING EQUATION IS USED FOR ALPHA BETWEEN -80 AND +1
$C N=F N C /((E X P(-A L P H A))+0.27)$
GO TO 20
C THE FOLLOWING EQUATION IS USED FOR ALPHA GREATER THAN +1
$10 \mathrm{CN}=\mathrm{FNC} * 0.752253 *(($ ALPHA*ALPHA+1.7)**0.75)
C COMPUTATION OF CP
$20 \quad C P=0$.
22 BETA=-EF/CAYT
IF (BETA.GT.1.) GO TO 30
IF (BETA.LE.-80.) GO TO 40
C THE FOLLOWING EQUATION IS USED FOR BETA BETWEEN -80 AND +1
$26 \quad \mathrm{CP}=\mathrm{FNV} /((\operatorname{EXP}(-\mathrm{BETA}))+0.27)$
GO TO 40
C THE FOLLOWING EQUATION IS USED FOR BETA GREATER THAN +1
$30 \mathrm{CP}=\mathrm{FNV} * 0.752253 *($ (BETA*BETA+1.7$) \star * 0.75)$
C COMPUTATION OF DI1
40 DI1=0.
IF (NAME1(1).EQ.6HDUMMY ) GO TO 60
POWER=(EF-EG+EN1) /CAYT
IF (POWER.GE.80.) GO TO 60
IF (POWER.LE.-80.) GO TO 50
DI1=DN1/(1.+(EXP (POWER)*DG1))
GO TO 60
50 DI1=DN1
C COMPUTATION OF DI2
60 DI2 $=0$.
IF (NAME2(1).EQ. 6HDUMMY) GO TO 80
POWER=(EF-EG+EN2)/CAYT
IF (POWER.GE.80.) GO TO 80
IF (POWER.LE.-80.) GO TO 70
$D I 2=D N 2 /(1 .+(E X P(P O W E R) * D G 2))$
GO TO 80
DI2=DN2
C COMPUTATION OF DI3

DI4=0.
If (NAME4(1).EQ.6HDUMMY ) GO TO 120
POWER=(EN4-EF)/CAYT
IF (POWER.GT.80.) GO TO 120
IF (POWER.LE.-80.) GO TO 110
DI4=DN4/(1.+(EXP (POWER)*DG4))
GO TO 120
110 DI4=DN4
C COMPUTATION OF DI5
120 DI5=0.
IF (NAMES(1).EQ.GHDUMMY ) GO TO 140
POWER=(EN5-EF)/CAYT
IF (POWER.GE.80.) GO TO 140
IF (POWER.LE.-80.) GO TO 130
DI5=DN5/(1.+(EXP (POWER)*DG5))
GO TO 140
DI5=DN5
TESTING TO SEE HOW CLOSE TO NEUTRALITY WE HAVE COME
THE PARAMETER TEST IS THE NET DENSITY OF RESIDUAL CHARGES
WHEN THE FERMI LEVEL IS AT ITS PRESENT POSITION
140 TEST $=(C N+D I 3+D I 4+D I 5)-(C P+D I 1+D I 2)$
RETURN
END

## SANDIA MATHEMATICAL PROGRAM LIBRARY

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ALBUQUERQUE, NEW MEXICO 87115
CONTROL DATA 6600 VERSION 4.5, 1 NOVEMBER 1971
MODIFIED TO RUN AT NBS BY D. KAHANER DIV 713
ABSTRACT
ZEROIN SEARCHES FOR A ZERO OF A FUNCTION $F(X)$ BETWEEN THE GIVEN VALUES B AND C UNTIL THE WIDTH OF THE INTERVAL ( $B, C$ ) HAS COLLAPSED TO WITHIN A TOLERANCE SPECIFIED BY THE STOPPING CRITERION, ABS (B-C) .LE. 2.*(RW*ABS (B) +AE).

DESCRIPTION OF ARGUMENTS
F - NAME OF THE REAL VALUED EXTERNAL FUNCTION. THIS NAME MUST BE IN AN EXTERNAL STATEMENT IN THE CALLING PROGRAM. F MUST BE A FUNCTION OF ONE REAL ARGUMENT.
B - ONE END OF THE INTERVAL ( $B, C$ ). THE VALUE RETURNED FOR B USUALLY IS THE BETTER APPROXIMATION TO A ZERO OF F.
C - THE OTHER END OF THE INTERVAL ( $B, C$ )
RE - RELATIVE ERROR USED FOR RW IN THE STOPPING CRITERION. If THE REQUESTED RE IS LESS THAN MACHINE PRECISION, THEN RW IS SET TO APPROXIMATELY MACHINE PRECISION.
AE - ABSOLUTE ERROR USED IN THE STOPPING CRITERION. IF THE GIVEN INTERVAL (B,C) CONTAINS THE ORIGIN, THEN A NONZERO VALUE ShOULD BE CHOSEN FOR AE.
IFLAG - RETURNS A STATUS OF THE RESULTS INDICATING WHICH OF THE FOLLOWING CONDITIONS HOLD.


E - NUMBER OF EVALUATIONS OF $F(X)$.LE. 500
$=1$ INDICATES NORMAL CASE. ALL CONDITIONS ABOVE HOLD. $=2$ INDICATES $F(B)=0$. CONDITION A MAY NOT HOLD. $=3$ INDICATES CONDITIONS A, B, C, AND E HOLD BUT D DOES NOT. ( $B, C$ ) PROBABLY CONTAINS A SINGULAR POINT OF F. $=4$ INDICATES CONDITIONS A AND E HOLD BUT B DOES NOT. A LOCAL MINIMUM OF $F(X)$ IN ( $B, C$ ) MAY HAVE BEEN FOUND. $=5$ INDICATES SEARCH WAS ABORTED WHEN CONDITION E FAILED.

REFERENCES

1. L F SHAMPINE AND H A WATTS, ZEROIN, A ROOT-SOLVING CODE, SC-TM-70-631, SEPT 1970.
2. T J DEKKER, FINDING A ZERO BY MEANS OF SUCCESSIVE LINEAR INTERPOLATION, *CONSTRUCTIVE ASPECTS OF THE FUNDAMENTAL THEOREM OF ALGEBRA*, EDITED BY B DEJON AND P HENRICI, 1969.
3. L F SHAMPINE AND $R$ C ALLEN, NUMERICAL COMPUTING--
1 IF (ABS(FC) .GE. ABS (FB)) GO TO 2
PERFORM INTERCHANGE
$A=B$
FA $=\mathrm{FB}$
$B=C$
$\mathrm{FB}=\mathrm{FC}$
$C=A$
$\mathrm{FC}=\mathrm{FA}$
$2 \mathrm{CMB}=0.5 *(\mathrm{C}-\mathrm{B})$
$A C M B=A B S$ (CMB)
TOL $=R W * A B S(B)+A E$
TEST STOPPING CRITERION
If (ACMB .LE. TOL) GO TO 10
CALCULATE NEW ITERATE IMPLICITLY AS B+P/Q
Where we arrange p .ge. 0.
the implicit form is used to prevent overflow.
$P=(B-A) \star F B$
$Q=F A-F B$
IF (P .GE. O.) GO TO 3
$P=-P$
$Q=-Q$
UPDATE A AND CHECK FOR SATISFACTORY REDUCTION
in the size of our bounding interval.
$3 A=B$
FA $=\mathrm{FB}$
$\mathrm{IC}=\mathrm{IC}+1$
IF (IC .LT. 4) GO TO 4
IF (8.*ACMB .GE. ACBS) GO TO 6
IC=0
ACBS $=A C M B$
TEST FOR TOO SMALL A CHANGE
4 IF (P .GT. ABS (Q)*TOL) GO TO 5

C INCREMENT BY TOLERANCE B=B+SIGN(TOL,CMB) GO TO 7

C
C ROOT OUGHT TO BE BETWEEN B AND $(C+B) / 2$. 5 IF (P .GE. CMB*Q) GO TO 6

C INTERPOLATE $B=B+P / Q$ GO TO 7

C
$6 B=0.5 *(C+B)$
BISECT
C
C HAVE COMPLETED COMPUTATION FOR NEW ITERATE B 7 FB=F(B)

IF (FB .EQ. O.) GO TO 11
KOUNT=KOUNT+1
IF (KOUNT .GT. 500) GO TO 15
C
C
DECIDE WHETHER NEXT STEP IS INTERPOLATION OR EXTRAPOLATION
IF (SIGN(1.0,FB) .NE. SIGN(1.0,FC)) GO TO 1
$C=A$
$\mathrm{FC}=\mathrm{FA}$
GO TO 1
C
C
C
FINISHED. PROCESS RESULTS FOR PROPER SETTING OF IFLAG
C
10 IF (FB*FC .GT. O.) GO TO 13
IF (ABS (FB) .GT. FX) GO TO 12
IFLAG $=1$ RETURN
11 IFLAG $=2$ RETURN
12 IFLAG $=3$ RETURN
13 IFLAG $=4$ RETURN
15 IFLAG $=5$ RETURN END

SUBROUTINE TO EVALUATE CARRIER MOBILITIES AND RELATED ITEMS
THIS SUBROUTINE CALLS SUBROUTINE SICI (SI,CI,X)
DIMENSION NAME1 (2), NAME2 (2), NAME3 (2), NAME4 (2), NAME5 (2)
COMMON NAME1,NAME2,NAME3,NAME4,NAME5
COMMON DN1,DN2,DN3,DN4,DN5,SUMTD,SUMTA
COMMON DI1,DI2,DI3,DI4,DI5
COMMON EN1,EN2,EN3,EN4,EN5
COMMON DG1,DG2,DG3,DG4,DG5
COMMON T, CN, CP, EG, EFME, EFMH, FNC, FNV, CAYT, TPOWR, Q, ALPHA, BETA
COMMON UD,UDN, ULN, UDP, ULP, SIGMA, RHO, RH
COMMON OUT8,OUT11,ISTAT
UPON RETURNING, ISTAT INDICATES THE STATUS OF THE COMPUTATIONS EACH DIGIT (POSITION) OF ISTAT IS USED INDIVIDUALLY

## ISTAT $=0$

DIEL $=4 * P I *(A B S O L U T E$ DIELECTRIC CONSTANT IN FARADS/METER)
RELATIVE DIELECTRIC CONSTANT AT 300 KELVIN $=11.7$
DUNLAP AND WATTERS, PHYS.REV. 92, 1396-1397 (1953)
TEMPERATURE DEPENDENCE CALCULATED FROM INDEX OF REFRACTION DATA CARDONA ET AL, J. PHYS. CHEM. SOLIDS. 8, 204-206 (1959) DIEL=1.2711E-9*EXP (7.8E-5*T)

SEE PAPERS BY LI AND THURBER, SSE 20, 609 AND LI, SSE 21, 1109
SUMID=DI1+DI2
SUMIA $=D I 3+D I 4+D I 5$
CION=DI1+DI2+DI3+DI4+DI5
$C N U T=D N 1+D N 2+D N 3+D N 4+D N 5-C I O N$
WE MUST GUARD AGAINST ZERO DIVISORS IN THE FOLLOWING COMPUTATIONS
SOME OF THESE ZERO DEVISORS WILL BE FLAGGED BY SETTING ISTAT
IF (CION.LE.O.) CION=1.
IF (CNUT.LE.O.) CNUT=1.
CALCULATION OF ELECTRUN MOBILITY
LATTICE SCATTERING (WITH CORRECTION FOR ELECT.-ELECT. SCATTERING) EQ FOR CORRECTION DEPENDS ON DONOR DENSITY
EQS FOR TEMPERATURE DEPENDENCE OF ULN FROM NORTON, ET AL.
SEE PAPER IN PHYS. REV. B8, 5632 (1973)
VALUE OF ULN AT 300 K FROM THURBER, ET AL. TO BE PUBLISHED IN JECS IF (SUMTD.GE.3.E17) GO TO 20
IF (T.GE.108.) GO TO 10
ULN $=1.89 E 7 \star T * *(-1.52) *(1 .-0.08 * S U M T D / 2 . E 17)$
GO TO 40
0 ULN $=7.98 E 8 * T * *(-2.32) *(1 .-0.08 * S U M T D / 2 . E 17)$
GO TO 40
IF (T.GE.108.) GO TO 30
ULN=1.89E7* (T** (-1.52)) *0.884
GO TO 40
ULN=7.98E8* (T** (-2.32) ) *0.884
ADD ON THE EFFECTS OF IONIZED IMPURITY SCATTERING
WE MUST ALLOW FOR THE FACT THAT SUMTD MIGHT VANISH IN CNSTAR EQ.
IF (SUMTD.LE.O.) CNSTAR=CN+CP
IF (SUMTD.LE.O.) GO TO 50
CNSTAR=CN+CP+(1.-SUMID/SUMTD)*SUMID
BN IS LOG TERM IN MODIFIED BROOKS-HERRING IONIZED IMPURITY MOB. EQ
$B N=6 * D I E L * M A S S *(1.3806 E-23) * * 2 * T * T /(P I * Q * Q * H B A R * H B A R * C N S T A R)$
WE MUST ALLOW FOR THE FACT THAT CNSTAR MIGHT VANISH IN EQ FOR BN
BN IS SET TO A LARGE NUMBER AND FIRST POSITION OF ISTAT
IS SET TO UNITY
IF (CNSTAR.LE.O.) BN=9.999999E19
IF (CNSTAR.LE.O.) ISTAT=ISTAT+1
IF (CNSTAR.LE.O.) GO TO 80
BN=1.14E24*DIEL*T*T/CNSTAR
IF BN IS SMALL, BORN APPROXIMATION IS NOT VALID. IN THIS CASE,
FIFTH POSITION OF ISTAT IS INCREMENTED.
If (BN-10.) 60,60,80
ISTAT=ISTAT+10000
IF (CION-1.0) 70,80,80
UDN=ULN
OUT8=UDN
GO TO 110
$\mathrm{GN}=\mathrm{ALOG}(\mathrm{BN}+1)-.\mathrm{BN} /(B N+1$.
CALCULATE GAMMA FOR EFFECT OF E-E SCATTERING ON ION. IMP. MOBILITY
IF (CNSTAR.LE.O.) GAMMA=0.632
IF (CNSTAR.LE.D.) GO TO 90
If (SUMID.LE.O.) GAMMA=0.432
IF (SUMID.GT.0.) GAMMA=(SUMID/CNSTAR)*(1.-EXP(-CNSTAR/SUMID))
IF (GAMMA.LT.0.432) GAMMA $=0.432$
UIN=GAMMA*7.3E17*TPOWR/(CION*GN)
IF (UIN.LE.O.) RATION=1.E6
IF (UIN.LE.O.) GO TO 100
RATION=6.*ULN/UIN
XN=SQRT (RATION)
COMBINE LATTICE AND IONIZED IMPURITY SCATTERING BY THE MIXED-
SCATTERING FORMULA OF DEBYE AND CONWELL, PHYS. REV. 93,
698-706 (1954). SUBROUTINE SICI PERFORMS THIS FUNCTION
CALL SICI (SI,CI,XN)
UDN=ULN* (1.0+RATION* (CI*COS (XN) +SIN(XN)*(SI-1.5707963)))
OUT8=UDN
ADD ON THE EFFECTS OF NEUTRAL IMPURITY SCATTERING
NEUTRAL IMPURITY MOBILITY AS PER ERGINSOY, PHYS REV 79,1013 (1950)
UNIS $=0.02 * P I * * 3 * Q * * 3 * M A S S /(5 * D I E L * C N U T * H * * 3)$
UNIS CONTAINS GEOMETRIC MEAN MASS WITH VALUE OF EFME/6**0.667
SEE BROOKS, ADV. IN ELECTRONICS AND ELECTRON PHYSICS 7, 161 (1955)
UNIS $=4.85 E 11$ *EFME/ (DIEL*CNUT)
SCLAR'S CORRECTION TO UNIS, SEE PHYS REV 104, 1559 (1956)
SEE ALSO PAPER BY LI AND THURBER, SSE 20, 609 (1977)
EI=0.215*EFME/( (DIEL/1.1121E-10)**2*CAYT)
UNIS=UNIS*0.82* (2*SQRT (1/EI) /3+SQRT (EI)/3.)
UDN=1/(1/UDN+1/UNIS)
that completes the computation of the electron mobility
CALCULATION OF HOLE MOBILITY
LATTICE SCATTERING WITH CORRECTION FOR HOLE-HOLE SCATTERING
EQ FOR ULP FOR T.LT. 72 FROM BRAGGINS, PHD THESIS,
SYRACUSE UNIVERSITY, 1975
EQ FOR ULP FOR T.GE. 72 FROM LUDWIG AND WATTERS,

| C | PHYS REV 101, 1699 (1956) |
| :---: | :---: |
|  | If (SUMTA.GE.3.E17) GO TO 130 |
|  | If (T.GE.72.) GO TO 120 |
| 118 | ULP $=1.6 E 7 * T * *(-1.54) *(1 .-0.08 * S U M T A / 2 . E 17)$ |
|  | GO TO 150 |
| 120 | ULP=2.3E9*T**(-2.7)*(1.-0.08*SUMTA/2.E17) |
|  | GO TO 150 |
| 130 | IF (T.GE.72.) GO TO 140 |
| 132 | ULP=1.6E7* (T** (-1.54) ) *0.884 |
|  | GO TO 150 |
| 140 | ULP=2.3E9* ( $T$ ** ( -2.7 ) ) *0.884 |
| C | ADD ON THE EFFECTS OF IONIZED IMPURITY SCATTERING |
| C | WE MUST ALLOW FOR THE FACT THAT SUMTA MIGHT VANISH IN CPSTAR EQ. |
| 150 | IF (SUMTA.LE.O.) CPSTAR=CN+CP |
|  | IF (SUMTA.LE.O.) GO TO 160 |
| 152 | CPSTAR $=C P+C N+(1 .-S U M I A / S U M T A) * S U M I A ~$ |
| C | BP IS LOG TERM IN BROOKS-HERRING IONIZED IMPURITY MOBILITY |
| C | $B P=6 * D I E L * M A S S *(1.3806 E-23) * * 2 * T * T /(P I * Q * Q * H B A R * H B A R * C P S T A R) ~$ |
| C | MASS FOR BP OF EACH BAND FROM LI, NBS SPECIAL PUBLICATION 400-47 |
| C | NO TEMPERATURE DEPENDENCE FOR MASS, 300 K VALUE USED |
| C | IS SET TO 1 |
| C | WE MUST ALLOW FOR THE FACT THAT CPSTAR MIGHT VANISH IN EQ FOR BP |
| C | BP IS SET TO A LARGE NUMBER AND THIRD POSITION OF ISTAT |
| 160 | If (CPSTAR.LE.O.) BP1=9.999999E19 |
|  | IF (CPSTAR.LE.O.) BP2=9.999999E19 |
|  | If (CPSTAR.LE.O.) BP3=9.999999E19 |
|  | If (CPSTAR.LE.0.) ISTAT=ISTAT+100 |
|  | If (CPSTAR.LE.O.) GO TO 190 |
| 162 | BP1=1.16E24*0.568*DIEL*T*T/CPSTAR |
|  | BP2=1.16E24*0.412*DIEL*T*T/CPSTAR |
|  | $\mathrm{BP} 3=1.16 \mathrm{E} 24 * 0.246 *$ IEL*T*T/CPSTAR |
| C | IF BP IS SMALL, BORN APPROXIMATION IS NOT VALID. IN THIS CASE, |
| C | FIFTH POSITION OF ISTAT IS INCREMENTED. |
|  | IF (BP1-10.) 170,170,190 |
| 170 | ISTAT=ISTAT +10000 |
|  | IF (CION-1.0) 180,190,190 |
| 180 | UDP $=$ ULP |
|  | OUT11=UDP |
|  | GO TO 220 |
| 190 | GP1=ALOG (BP1+1.)-BP1/ (BP1+1.) |
|  | $\mathrm{GP2}=\mathrm{ALOG}(\mathrm{BP} 2+1)-.\mathrm{BP} 2 /(\mathrm{BP} 2+1$. |
|  | GP3 $=$ ALOG (BP3+1.)-BP3/(BP3+1.) |
| C | UIP $=0.01 *(2 * * 3.5) *$ DIEL*DIEL*SQRT (MD)* $(1.38 \mathrm{E}-23 * T) * * 1.5 /$ |
| C | ( (PI**1.5) *Q*Q*Q*MC*CION*GP) |
| 192 | UIP1 $=2.66 E 35 *$ I IEL *DIEL*TPOWR*SQRT (0.568) / (0.448*CION*GP1) |
|  | UIP2 $=2.66 E 35 *$ DIEL*DIEL*TPOWR*SQRT (0.412) / (0.532*CION*GP2) |
|  | UIP3 $=2.66 E 35 *$ I 1 L * D IEL*TPOWR*SQRT (0.246) / (0.253*CION*GP3) |
| C | WEIGHT INDIVIDUAL MOBILITIES BY HOLE DENSITY IN THAT BAND |
| 196 | UIP $=($ UIP1 + UIP $2 *(0.412 / 0.568) \star * 1.5+$ UIP $3 * E X P(-0.044 / C A Y T) *(0.246 / 0.5$ |
|  | 268)**1.5)/(1.+(0.412/0.568)**1.5+EXP (-0.044/CAYT)*(0.246/0.568)**1 |
|  | 3.5) |
| C | CALCULATE GAMMA FOR EFFECT OF H-H SCATTERING ON ION. IMP. MOBILITY |
|  | IF (CPSTAR.LE.O.) GAMMA $=0.632$ |

```
    IF (CPSTAR.LE.O.) GO TO 200
IF (SUMIA.LE.O.) GAMMA=0.432
IF (SUMIA.GT.0.) GAMMA=(SUMIA/CPSTAR)*(1. -EXP(-CPSTAR/SUMIA))
    IF (GAMMA.LT.0.432) GAMMA=0.432
UIP=GAMMA*UIP
IF (UIP.LE.O.) RATIOP=1.E6
IF (UIP.LE.O.) GO TO 210
C SCLAR'S CORRECTION TO UNIS, SEE PHYS REV 104, 1559, (1956)
```

RETURN

```
END
```

C THIS ROUTINE COMBINES LATTICE AND IONIZED MOBILITY SCATTERING ACCORDING TO THE MIXED-SCATTERING FORMULA OF DEBYE AND CONWELL, PHYS. REV. 93, 693-706 (1954)

TEST ARGUMENT RANGE
$Z=A B S(X)$
IF (Z-4.) 10,10,50
$Z$ IS NOT GREATER THAN 4.
$10 \quad Y=Z * Z$
$S I=X *((()(C .97942154 E-11 \star Y-.22232633 E-8) \star Y+.30561233 E-6) \star Y-.283414$ 260E-4) *Y+. $16666582 E-2) \star Y-.55555547 E-1) \star Y+1$.
TEST FOR LOGARITHMIC SINGULARITY
If (Z) 30,20,30
20 CI=-1.E38
RETURN
$30 C I=0.57721566+A L O G(Z)-Y *((C((-.13869851 E-9 * Y+.26945842 E-7) \star Y-.3095$ $22207 E-5) * Y+.23146303 E-3) \star Y-.10416642 E-1) * Y+.24999999)$
RETURN
C $\quad Z$ IS GREATER THAN 4.
$50 \quad \mathrm{SI}=\operatorname{SIN}(\mathrm{Z})$
$Y=\cos (Z)$
$Z=4.1 Z$
$U=(()((()(.40480690 E-2 \star Z-.022791426) * Z+.055150700) \star Z-.072616418) * Z$ $2+.049877159) * Z-.33325186 E-2) * Z-.023146168) * Z-.11349579 E-4) * Z+.0625$ 300111)*Z+.25839886E-9
$V=((C((C((-.0051086993 * Z+.028191786) * Z-.065372834) * Z+.079020335) *$ $2 Z-.044004155) * Z-.0079455563) * Z+.026012930) * Z-.37640003 E-3) * Z-.0312$ 324178)*Z-.66464406E-6)*Z+. 25000000

CI=Z* (SI*V-Y*U)
$S I=-Z *(S I * U+Y * V)+1.5707963$
$C$ TEST FOR NEGATIVE ARGUMENT
IF (X) $60,40,40$
$X$ IS LESS THAN -4.
$C \quad \begin{array}{ll}C & X \\ 60 & S I=-S I\end{array}$
RETURN
END

### 5.1 Data Cards Used to Generate Output Listings

The output examples to follow illustrate a no-option run, the DOUBLE ON format, the DOLOOP XX option, and the CONSTANTS option. Following is a listing of the complete deck of dopant state data and control cards that were used to generate these output examples. Lines separate the card sets for each example.

| PHOSPHORUS <br> DUMMY <br> DUMMY <br> BORON <br> DUMMY | $1.00000 E 15$ | 0.045 | 2. |
| :--- | :--- | :--- | :--- |
| DOUBLE ON <br> PHOSPHORUS <br> DUMMY <br> DUMMY | $1.00000 E 18$ | 0.045 | 2. |
| BORON <br> DUMMY <br> DOUBLE OFF | $1.00000 E 13$ | 0.045 | 4. |
| DOLOOP AZ <br> PHOSPHORUS <br> DUMMY <br> DUMMY <br> BORON <br> DUMMY | 1.00000 .00015 |  |  |


5．3 Illustration of the DOUBLE ON Option Output
ELECTRICAL PROPERTIES OF SILICCN
$\begin{array}{ll}\text { DCPANT STATES FCR THIS FUN } \\ & \\ \text { OOPANT } & \text { DENS } 1 T Y \\ \text { PHCSPHCRLS } & 1.000+18 \\ \text { BORON } & 1.000+13\end{array}$
$\begin{array}{cl}\text { DCPANT STATES FCR THIS FUN } \\ & \\ \text { OOPANT } & \text { DENS } 1 T Y \\ \text { PHCSPHCRLS } & 1.000+18 \\ \text { BORON } & 1.000+13\end{array}$
$\begin{array}{ll}\text { DCPANT STATES FCR THIS FUN } \\ \text { ODPANT } & \\ \text { DENS } 1 \text { TY } \\ \text { PHCSPHCRLS } & 1.000+18 \\ \text { BORON } & 1.000+13\end{array}$
$\begin{array}{ll}0 & 0 \\ 0 \\ 4 \\ 8 \\ 8 \\ 8\end{array}$
$0000 \cdot z$
ヘコロロヨNヨ9ヨ0
2.0000
4.0000
$\stackrel{L}{2}$
$\vdots$
1
0
0
0


|  | n） | F1 N |
| :---: | :---: | :---: |
| 」 | $=0$ | － 0 |
| $\underline{8}$ | $\stackrel{+}{0}$ | ＋${ }^{+}$ |
| $\stackrel{5}{5}$ | $\bigcirc$ | $\bigcirc$ |
| 3 | $\bigcirc 0$ | $\bigcirc$ |
| 2 | $\cdots$ | $\cdots+$ |


| $n$ |
| :---: |
| + |
| + |
| 0 |
| 0 |
| 0 |
| 0 |
| 0 |
| -0 |


$\begin{array}{lll}N & m & n \\ 0 & \vdots & + \\ + & 0 & 0 \\ 0 & 0 \\ \infty & 0 & 0 \\ 0 & \vdots & 0 \\ \dot{0} & - & +\end{array}$


$n$
0
+
0
0
0
0
$\vdots$
$\vdots$

$m$
$\cdots$
+
$\vdots$
0
0
$\vdots$
$\vdots$
$\vdots$
$n$
0
0
0
$n$
0
0
0
 $4.613+02$
$1.000+12$
$4.536+02$


0
u
N
$\mathbf{z}$
$\mathbf{0}$
A1 10

+
+
+
$\sim$
$N$
$\vdots$
$\vdots$

| + |
| :--- |
| 0 |
| + |
| + |
| 0 |
| 0 |
| 0 |


$m$
0
+
+
+
$\vdots$
$\vdots$
$5.553+03$

| $m$ |
| :--- |
| $\mathbf{O}$ |
| + |
| $\mathbf{N}$ |
| $\infty$ |
| $\vdots$ |
| $\vdots$ |
| $\vdots$ |

$m$
0
$\vdots$
0
$\omega$
$\dot{m}$
$m$
0
+
$\mathbf{N}$
$\mathbf{N}$
$\vdots$
$\dot{N}$
$\dot{N}$


| に |
| :--- |
| $\stackrel{0}{+}$ |
| + |
| 0 |
| 0 |
| + |
| $\vdots$ |
| $\vdots$ |


| $๑$ | $n$ | 0 | 0 | $\bigcirc$ |
| :---: | :---: | :---: | :---: | :---: |
| $\bigcirc$ | $\bigcirc$ | $\bigcirc$ | $\bigcirc$ | $\stackrel{+}{+}$ |
| $\stackrel{+}{0}$ | $\stackrel{+}{\text {＋1 }}$ | $\stackrel{+}{\square}$ | $\stackrel{+}{0}$ | $\stackrel{+}{0}$ |
| $\stackrel{9}{0}$ | $\bigcirc$ | $\stackrel{\square}{4}$ | N | $\stackrel{8}{8}$ |
| $\cdots$ | $\cdots$ | $\sim$ | $\cdots$ | － |
| $\rightarrow$ | － | $\rightarrow$ | － | $\rightarrow$ |

$\begin{array}{ll} \pm & 0 \\ 0 & 0 \\ + & + \\ 0 & N \\ 0 & 0 \\ 0 & 0 \\ 0 & \infty\end{array}$ $\infty$
+
+
0
0
$\vdots$

$m$
$\cdots$
+
+
0
0
0
$\vdots$
$\vdots$





$\pm$
$\pm$
$\pm$
+0
0
0
$\sim$





$a$
$N$
+
+
+
$m$
0
0
$\vdots$
$\vdots$
$N$
0
+
+
$N$
0
0
-
$1 \cdot 115+02$
$\begin{array}{rr}-1 \\ 0 & 0 \\ + \\ + \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ \sim & -1\end{array}$


$\begin{array}{ll}-3 & m \\ o & 0 \\ + & + \\ N & 0 \\ 0 & 0 \\ 0 & 0 \\ m & 0\end{array}$



$8.167+00$
$\begin{array}{ll}\circ & m \\ 0 & 0 \\ + \\ + \\ \text { N } \\ \text { N } \\ 0 & m \\ \text { n } & \text { m }\end{array}$

$\begin{array}{ll}0 & 0 \\ 0 & 0 \\ + & + \\ 0 & 0 \\ 0 & n \\ ! & n \\ 0 & - \\ 0 & -1\end{array}$
$\begin{array}{ll}\infty & 0 \\ 0 & 0 \\ + \\ 0 & + \\ 0 & \\ 0 & 0 \\ 0 & 0 \\ i & 0 \\ i\end{array}$
+
+
+
0
-1
$\sim$
$\stackrel{1}{n}$
$i$
$-1.736+04$


$\begin{array}{ll}m & n \\ 0 & 0 \\ + \\ m & + \\ 0 & 0 \\ & 0 \\ \vdots & -1\end{array}$
$m$
0
0
0
+
$0_{0}$
$N$
0
0
0
$\dot{m}$
1
1
$-2.700+03$
$9.790+04$

COND．MOB
SIGMA
$20+55 \varepsilon^{-\varepsilon}$
$\varepsilon 0-\angle \succcurlyeq I^{\circ} 9$
$20+Z 92^{\circ} E$

$3.28 E+02$
$1.30 \in-02$
$3.29 \epsilon+02$
$1.898-02$

3． $311+02$
4． $003-02$

$3.312+02$
$8.43 \epsilon-02$
$3.305+02$
$1.224-01$

ENERGY（CALC．）
.0286
.0090
ENERGY（CALC．）

3． $314+02$
$a$
2
0
0
0
ENERGY（1 NPUT）
.0450
$E F$
$K T / Q$
$1.1310 \equiv 2$
$3.6193-04$
$1.197-13$
.246486
1．176＋14
$1.710+14$
$2.481+14$
.143844
$\pm$
$\vdots$
$\vdots$
0
0
$n$
0
$\dot{m}$ .144425 $5.208+14$ $7.546+14$
.145978

\[

\]


238.0952
$4.801+05$
50.0000
$-9.836+09$

$$
\begin{array}{r}
1.141130 \\
2.2677-03
\end{array}
$$

$$
\begin{aligned}
& 2.312+15 \\
& .149547
\end{aligned}
$$


$\begin{array}{ll}0 & 0 \\ 0 & - \\ 0 & + \\ 0 & + \\ 0 & 0 \\ 0 & 0 \\ + & 0 \\ & 1\end{array}$
44.0000
$-2.991+05$
$\begin{array}{ll}\circ & 0 \\ 0 & 0 \\ 0 & t \\ 0 & 0 \\ 0 & 0 \\ 0 & 0\end{array}$
40.0000
$-5.964+09$
38.0000
$-1.441+10$
$\begin{array}{ll}0 & 0 \\ 0 & 0 \\ 0 & + \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ m & 0\end{array}$
34.0000
$-1.698+12$

TEMP
品
4.2000
1.155681
20.0060
1.155867
20.8333
$1.1558 \in 6$
$21.73 ¢ 1$
$1.15586 \rightrightarrows$
22.7273
1.155858
23.8055
-1
0
$n$
$n$
0
$\vdots$
25.0000
1.155841
26.3158
1.155827
27.7778
1.155809
$29.411 \varepsilon$
$1.1557 \varepsilon 5$
31.2500
1.155752

$$
\begin{array}{r}
1.141243 \\
2.1543-03
\end{array}
$$

$$
\begin{array}{r}
1.140830 \\
2.5345-03
\end{array}
$$

$$
\begin{aligned}
& 1.590+15 \\
& .148151
\end{aligned}
$$

$$
\begin{aligned}
& \begin{array}{l}
n \\
\pm \\
+ \\
0 \\
0 \\
\vdots \\
\vdots
\end{array} \\
& \begin{array}{l}
1.094+15 \\
.146976
\end{array}
\end{aligned}
$$

| 33.3333 | 30.0000 | 1.140355 | $4.930+15$ | $3.270+02$ | $-1.266+03$ | $3.872+00$ | $4.932+15$ |  |  | $1.000+13$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1.155709 | $-1.191+11$ | 2．8724－03 | ． 153140 | 2．583－01 | $8.094+04$ | 2．694＋03 | 3．270402 | 7．226＋04． | $2.367+03$ | 4.333 .02 |
| 35.7143 | 28.0000 | 1.140102 | 7．223＋15 | 3．240＋02 | $-8.641+02$ | $2.667+00$ | $7.230+15$ |  |  | $1.000+13$ |
| 1．1556E1 | 3．335＋12 | 3．0776－03 | ． 155492 | 3．750－01 | $7.288+04$ | 2．189＋03 | $3.240+02$ | $6.457+04$ | $1.922+03$ | $4.205+02$ |
| 38．4615 | 26.0000 | 1.139737 | $1.062+16$ | $3.200+02$ | $-5.876+02$ | $1.836+00$ | $1.063+16$ |  |  | $1.000+13$ |
| 1.155574 | $1.730+12$ | 3．3143－03 | ． 158368 | $5.446-01$ | $6.511+04$ | $1.787+03$ | $3.200+02$ | 5．797＋04 | $1.567+03$ | $4.060+02$ |
| 41.6667 | 24.0000 | 1.139278 | $1.567+16$ | 3．152＋02 | $-3.984+02$ | 1．264＋00 | 1．569＋16 |  |  | $1.000+13$ |
| 1.155469 | $5.745+10$ | 3．5905－03 | ． 161915 | 7．511－01 | $5.765+04$ | $1.465+03$ | 3．152＋02 | $5.124+04$ | $1.284+03$ | $3.900+02$ |
| 45.4545 | 22.0000 | 1.138689 | $2.322+16$ | $3.095+02$ | $-2.688+02$ | ع．686－01 | $2.325+16$ |  |  | $1.000+13$ |
| 1．155ここ6 | $2.242+12$ | 3．9170－03 | ． 166363 | $1.151+00$ | $5.051+04$ | $1.209+03$ | $3.095+02$ | $4.482+04$ | $1.058+03$ | 3．729＋02 |
| $\leq 0.0000$ | 20.0000 | 1.137919 | 3．455＋16 | 3．033＋02 | $-1.806+02$ | 5．956－01 | 3．459＋16 |  |  | $1.000+12$ |
| 1．15512s | $1.290+12$ | 4．3086－03 | ． 172063 | $1.675+00$ | $4.370+04$ | $1.005+03$ | $3.033+02$ | $3.870+04$ | $8.777+02$ | 3．551＋02 |
| Eヒ．55se | 18.0000 | 1.136885 | 5．166＋16 | 2．570＋02 | $-1.208+02$ | 4．059－01 | 5．172＋16 |  |  | $1.000+13$ |
| 1.154840 | $5.057+11$ | 4．7874－03 | ． 179550 | $2.458+00$ | $3.723+04$ | 8．419＋02 | $2.970+02$ | 3．290＋04 | 7．335＋02 | $3.373+02$ |
| 62.5000 | 16.0000 | 1．135452 | 7．761＋16 | 2．511＋02 | $-8.042+01$ | 2．763－01 | 7．768＋16 |  |  | $1.000+13$ |
| $1.1544=2$ | $1.652+12$ | £．3858－03 | ． 189694 | $3.615+00$ | 3．113＋04 | 7．119＋02 | $2.911+02$ | $2.744+04$ | $6.184+02$ | $3.201+02$ |
| 71.4286 | 14.0000 | 1.133366 | 1．171＋17 | $2.866+02$ | $-5.328+01$ | 1．859－01 | 1．171＋17 |  |  | $1.000+13$ |
| 1.153786 | $-2.674+11$ | 6．1552－03 | －203995 | $5.378+00$ | $2.541+04$ | $6.089+02$ | $2.866+02$ | 2．234＋04 | 5．267＋02 | $3.045+02$ |
| 77．0C60 | 12.9870 | 1.131972 | 1．444＋17 | $2.852+02$ | －4．321＋01 | 1．515－01 | $1.445+17$ |  |  | $1.000+13$ |
| $1.1533 \equiv 5$ | $-4.078+13$ | 6．6353－03 | ． 213633 | $6.600+00$ | $2.267+04$ | $5.654+02$ | $2.852+02$ | $1.254+04$ | $4.851+02$ | $2.966+02$ |
| 83．33ミ3 | 12.0000 | $1.1302 \leq 2$ | $1.773+17$ | $2.84 \varepsilon+02$ | $-3.519+01$ | 1．236－01 | $1.773+17$ |  |  | $1.000+13$ |
| 1．152773 | $-6.550+11$ | 7．1811－03 | ． 225213 | $8.092+00$ | $2.010+04$ | 5．282＋02 | $2.848+02$ | $1.498+04$ | $4.484+02$ | $2.892+02$ |
| so．sos 1 | 11.0000 | 1．128037 | 2．181＋17 | $2.856+02$ | $-2.862+01$ | 1．002－01 | 2．182＋17 |  |  | $1.000+13$ |
| 1.152034 | $2.107+12$ | 7．833s－03 | ． 239965 | 9．580＋00 | $1.761+04$ | $4.954+02$ | $2.856+02$ | 1．184＋04 | $4.143+02$ | $2.820+02$ |
| 100.0000 | 10.0000 | 1.125161 | $2.683+17$ | $2.875+02$ | －2．326＋01 | ع．078－02 | 2．682＋17 |  |  | $1.000+13$ |
| $1.1510 \leq 3$ | $-3.649+11$ | 8．6173－03 | ． 258918 | $1.23 \varepsilon+01$ | $1.524+04$ | $4.673+02$ | $2.879+02$ | $9.156+03$ | 3．838＋02 | $2.754+02$ |
| 111.1111 | 5.0000 | 1.121334 | 3．293＋17 | 2． $520+02$ | －1．895＋01 | 6．491－02 | $3.292+17$ |  |  | $1.000+13$ |
| 1.149722 | $-8.719+11$ | 9．5748－03 | ． 283882 | $1.541+01$ | $1.266+04$ | $4.429+02$ | $2.920+02$ | $6.889+03$ | 3． $556+02$ | $2.690+02$ |
| 125.0000 | 8.0000 | 1.11 6086 | $4.025+17$ | 2．571＋02 | －1．551＋01 | 5．219－02 | $4.025+17$ |  |  | $1.000+13$ |


| $1 \cdot 1478 \in 2$ | $4 \cdot 933+13$ | 1．0772－02 | ． 317754 |  | 1．S $16+01$ | $9 \cdot 630+03$ | $4 \cdot 201+02$ | $2.971+02$ | $5.013+03$ | $3.294+02$ | $2.625+02$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 142．8571 | 7.0000 | 1.108624 | 4．889＋17 |  | 3．04 $\mathbf{4}+02$ | －1．277＋01 | 4．196－02 | $4 \cdot 888+17$ |  |  | $1.000+13$ |
| 1.145170 | $-7.813+12$ | $1.2310-02$ | －365459 |  | $2.38 \geq+01$ | 7．065＋03 | $4.010+02$ | $3.042+02$ | 3．495＋03 | $3.041+02$ | $2.552+02$ |
| 166．C6E7 | 6.0000 | 1.057527 | $5.871+17$ | 4．099－15 | 3．12s＋02 | $-1.063+01$ | 3．397－02 | $5 \cdot 870+17$ |  |  | $1 \cdot 000+13$ |
| 1．1410¢8 | $-1.298+13$ | 1．4362－02 | ． 435719 |  | 2．544＋01 | 4．940＋03 | 3．846＋02 | 3．129＋02 | 2． $305+03$ | 2．782＋02 | $2 \cdot 454+02$ |
| 200.0000 | 5.0000 | 1.080042 | $6 \cdot 930+17$ | 5．362－09 | 3． $20 \epsilon+02$ | －9．006＋00 | 2．809－02 | 6．929＋17 |  |  | $1.000+13$ |
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A FORTRAN program has been presented for calculating the electrical properties of silicon containing five dopant states. The charge-balance equation is solved to arrive at the Fermi energy which determines the carrier densities. An effective conductivity mobility is calculated for both electrons and holes, taking into account the significant scattering mechanisms, and then the resistivity is computed from the mobilities and carrier densities. An attempt has been made to include in the algorithm the temperature and dopant density dependence of as many parameters as possible. In some cases (e.g., the temperature dependence of the indirect energy gap of silicon), there are numerous experimental results in the literature [27]. In cases where there is significant disagreement in the literature (e.g., the variation of dopant activation energy with dopant density), there is room for improvement. In a few cases where little or nothing is known (e.g., the variation of the Hall scattering factor with temperature and dopant density), no attempt has been made to include these effects. Therefore, the user of this program is urged to review the literature regularly for additional or more comprehensive measurements that would improve the accuracy of the computed results. The authors invite any suggestions and comments in this regard.

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28. Submitting organization and address

National Bureau of Standards
Electron Devices Division
Washington, DC 20234
12. Technical contact(s) and phone
R. D. Larrabee
(301) 921-3625
W. R. Thurber
(301) 921-3625
W. M. Bullis
(301) 921-3786
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