

NBS SPECIAL PUBLICATION 400-63

U.S. DEPARTMENT OF COMMERCE / National Bureau of Standards

Semiconductor Measurement Technology:

A FORTRAN Program for Calculating the Electrical Parameters of Extrinsic Silicon

100 - 63

NATIONAL BUREAU OF STANDARDS

The National Bureau of Standards' was established by an act of Congress on March 3, 1901. The Bureau's overall goal is to strengthen and advance the Nation's science and technology and facilitate their effective application for public benefit. To this end, the Bureau conducts research and provides: (1) a basis for the Nation's physical measurement system, (2) scientific and technological services for industry and government, (3) a technical basis for equity in trade, and (4) technical services to promote public safety. The Bureau's technical work is performed by the National Measurement Laboratory, the National Engineering Laboratory, and the Institute for Computer Sciences and Technology.

THE NATIONAL MEASUREMENT LABORATORY provides the national system of physical and chemical and materials measurement; coordinates the system with measurement systems of other nations and furnishes essential services leading to accurate and uniform physical and chemical measurement throughout the Nation's scientific community, industry, and commerce; conducts materials research leading to improved methods of measurement, standards, and data on the properties of materials needed by industry, commerce, educational institutions, and Government; provides advisory and research services to other Government agencies; develops, produces, and distributes Standard Reference Materials; and provides calibration services. The Laboratory consists of the following centers:

Absolute Physical Quantities² — Radiation Research — Thermodynamics and Molecular Science — Analytical Chemistry — Materials Science.

THE NATIONAL ENGINEERING LABORATORY provides technology and technical services to the public and private sectors to address national needs and to solve national problems; conducts research in engineering and applied science in support of these efforts; builds and maintains competence in the necessary disciplines required to carry out this research and technical service; develops engineering data and measurement capabilities; provides engineering measurement traceability services; develops test methods and proposes engineering standards and code changes; develops and proposes new engineering practices; and develops and improves mechanisms to transfer results of its research to the ultimate user. The Laboratory consists of the following centers:

Applied Mathematics — Electronics and Electrical Engineering² — Mechanical Engineering and Process Technology² — Building Technology — Fire Research — Consumer Product Technology — Field Methods.

THE INSTITUTE FOR COMPUTER SCIENCES AND TECHNOLOGY conducts research and provides scientific and technical services to aid Federal agencies in the selection, acquisition, application, and use of computer technology to improve effectiveness and economy in Government operations in accordance with Public Law 89-306 (40 U.S.C. 759), relevant Executive Orders, and other directives; carries out this mission by managing the Federal Information Processing Standards Program, developing Federal ADP standards guidelines, and managing Federal participation in ADP voluntary standardization activities; provides scientific and technological advisory services and assistance to Federal agencies; and provides the technical foundation for computer-related policies of the Federal Government. The Institute consists of the following centers:

Programming Science and Technology - Computer Systems Engineering.

¹Headquarters and Laboratories at Gaithersburg, MD, unless otherwise noted; mailing address Washington, DC 20234. ²Some divisions within the center are located at Boulder, CO 80303.

NATIONAL BUREAU OF STANDARDS LIBRARY NOV 2 4 1980 MUL A Circ Q JO .UST MO 400 65 1430

Semiconductor Measurement Technology:

A FORTRAN Program for Calculating the Electrical Parameters of Extrinsic Silicon

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

Electron Devices Division Center for Electronics and Electrical Engineering National Engineering Laboratory National Bureau of Standards 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

Issued October 1980

SA SA

Library of Congress Catalog Card Number: 80-600158

National Bureau of Standards Special Publication 400-63 Nat. Bur. Stand. (U.S.), Spec. Publ. 400-63, 54 pages (Oct. 1980) CODEN: XNBSAV

> U.S. GOVERNMENT PRINTING OFFICE WASHINGTON: 1980

For sale by the Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. 20402 Price \$3.75 (Add 25 percent for other than U.S. mailing)

Table of Contents

Page

Abst	tract	• • •	• • •	• •	•	••	• •	٠	•	•	•	•	•	•	•	• •	•	٠		•	•	•	٠	•	1
1.	Intro	oductic	on	• •	٠	••	• •	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	•	1
2.	Desci	iption	of P	rogra	am (Opei	ati	.on	•	•	•	•	•	•	•	• •	•	•	•	•	•	•	•	•	3
	2.1 2.2 2.3	Option 2.1.1 2.1.2 2.1.3 2.1.4 2.1.5 Warnin	DOUBI DOUBI CONST DOLOG STOP	LE ON LE OF FANTS OP X2 Erro	N FF S X P Dr N	ARG	(1) sage	A	RG	(2)	•	•	•	•	•			• • • •	5 5 6 7 8 8						
3.	Theor	ry and	Metho	d of	Cor	nput	ati	.on	•	•	•	•	•	•	•	• •	•	•	•	•	•	•	•	•	10
	3.1 3.2	Locati Comput	on of ation	the of (Fei Cari	rmi riez	Lev Mo	el bi	lit	ie	·	an	• đ 1	Re	lat	zed	· I P	ara	am	• et@	• ers	•	•	•	10 14
4.	Annot	ated P	rogram	n Lis	stir	ng	• •	•	•	•	•	•	•	•	• •		•	•	•	•	•	•	•	•	19
5.	Illus	strativ	e Out	put I	Data	a Ca	rds	a	nd	Ex	am	pl	es		•	•	•	٠	•	•	•	٠	•	•	36
	5.1 5.2 5.3 5.4 5.5	Data C Illust Illust Illust Illust	ards (ration ration ration ration	Used n of n of n of n of	to a l the the	Ger No-C e DC e DC e CC	pera Opti OUBL OLOO	on E P	O OU MC XX IS	itp itp Op Op Op	out out oti oti	on on	is O O	tin • utj utj	ngs out out		•	• • •	• • •	• • •	• • •	• • •	• • •	• • •	36 37 38 41 45
6.	Concl	usions		• •	•	•••	• •	•	•	•	•	•	•	•	•	• •	•	•	•	•	•	•	•	•	46
Ackı	nowled	lgments	• •	• •	• •	• •	• •	•	•	•	٠	•	•	•		•	•	•	•	•	•	•	•	•	46
Refe	erence	es		•••	•	•••	•••	•	•	•	•	•	•	•	•	• •	•	•	•	•	•	•	•	•	46
							Lis	st (of	Та	bl	es													

		Pa ge
1.	Symbols Used in Mobility Formulas	15
2.	Formulas for Calculating Electron Mobility	16
3.	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.

Semiconductor Measurement Technology: 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

1

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} 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

2

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.
- 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 Al, 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, 2Fl0.4, 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:

- the position of the Fermi level with respect to the valence band in electron volts,
- the density of electrons in the conduction band in reciprocal cubic centimeters,
- the density of holes in the valence band in reciprocal cubic centimeters,
- 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/(temperature). The incremental values of 1000/(temperature) are specified independently in each of the three temperature regions. As presently written, the temperature following 4.2 K is 20 K (1000/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/T =Above 300 K, the temperature is increased in intervals of 1000/T = 0.5. 1. The FORTRAN parameter RUNNO keeps track of things as follows:

RUNNO = 1, 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.).

2.1 OPTIONS

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, 2F10.4), 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 ON 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.

A run is herein defined as the evaluation of one set of five dopant state data cards over the full temperature range.

- 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.
- 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 CON-STANTS 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/(temperature) in inverse kelvin,
- 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,
- the upper limiting mobility of electrons in the conduction band set by lattice scattering in square centimeters per volt-second,
- 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 Dl, D2, Al, A2, and A3. If anything else appears in the XX 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(1) 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, 2F10.4), 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, BN, 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 = XX ERROR IN N MAY EXCEED 1 PERCENT

In this warning message, XX 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 XX > -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 = XX 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 = 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 <u>TEST</u> and the subroutine <u>ZEROIN</u> are used for finding the position of the Fermi level, and the subroutines <u>MOB</u> and <u>SICI</u> 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 <u>IF</u> statements that test alphanumeric variables for machines that do not store six alphanumeric characters per word.

9

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 <u>TEST</u> is a measure of how precisely the algorithm has located the position of the Fermi level to obtain charge neutrality.

```
TEST = (Net negative charge) - (Net positive charge)TEST = (CN + DI3 + DI4 + DI5) - (CP + DI1 + DI2) (140)*
```

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

CN, electrons in the conduction band, CP, holes in the valence band, DI1, ionized donor species 1,

The statement numbers in this section refer to the function <u>TEST</u> unless otherwise indicated.

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 Fermi-Dirac integral [5]:

$$n = N \left[\exp(-\eta) + 0.27 \right]^{-1}$$
(8,26)

for values of η in the range from -80 to +1,

$$n = 0.752253 N (\eta^2 + 1.7)^{3/4}$$
(10,30)

for values of η greater than +1, and

$$n = 0$$
 (2,20)

for values of η less than -80. In these equations, n is the electron or hole density, N is the density of states in the appropriate band, $\eta = q(E_F - E_g)/kT$ for electrons (4), and $-qE_F/kT$ for holes (22), E_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 kT/q is the voltage equivalent of the temperature (353 of Main Program).

The density of states is given by

$$N = 2(2\pi k m_{o}/h^{2})^{3/2} m^{*3/2} T^{3/2}$$
$$= 4.829 \times 10^{15} m^{*3/2} T^{3/2},$$

(354,355) Main Program

where m^* is the effective mass of the appropriate carrier relative to the free electron mass, m_0 . The relative electron effective mass, m_e^* , is given by $[7]^{\dagger}$

$$m_{e}^{*} = 1.0627 - 1.61708 \times 10^{-4} \text{T} + 6.83008 \times 10^{-6} \text{T}^{2} - 3.32013 \times 10^{-8} \text{T}^{3} + 8.04032 \times 10^{-11} \text{T}^{4} - 9.66067 \times 10^{-14} \text{T}^{5} + 4.54649 \times 10^{-17} \text{T}^{6}$$

(350) Main Program

and the relative hole effective mass, m^{*}_b, is given by [7]

[†]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.

$$m_{h}^{*} = 0.590525 - 5.23548 \times 10^{-4} T + 1.85678 \times 10^{-5} T^{2} - 9.67212 \times 10^{-8} T^{3} + 2.30049 \times 10^{-10} T^{4} - 2.596730 \times 10^{-13} T^{5} + 1.11997 \times 10^{-16} T^{6} .$$
(352) Main Program

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]:

$$E_{g} = 1.15556 + 3.23741 \times 10^{-5}T - 8.7011 \times 10^{-7}T^{2} + 9.95401 \times 10^{-10}T^{3}$$

- 3.80977 x 10⁻¹³T⁴.

(356) Main Program

The density of ionized impurities is computed from the following:

$$N_{i} = N_{t} [1 + g \exp(\Delta)]$$
 (40 ff)

where N_t is the total density of the dopant impurity, g is the degeneracy factor, and $\Delta = q(E_F - E_g + E_A)/kT$ for donor states and $q(E_A - E_F)/kT$ 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:

- 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.
- 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.
- 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,
- 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 x 10^{18} cm⁻³ regardless of the initial activation energy, E_{A0} . 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 x 0.045, where 0.045 is the phosphorus activation energy, is fixed at 0.36. Thus, since E_{A0} 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

$$E_{A} = E_{A0} - 0.36 \left(\frac{1}{2} + \frac{a^{*}}{r_{d}}\right) \exp\left(-r_{d}/a^{*}\right) - \alpha N_{2}^{1/3}$$

(70 ff) Main Program

where E_{A0} is the activation energy for low densities of the dopant, $r_d = [3/(4\pi N_1)]^{1/3}$ is the average distance between the dominant dopant atoms of a given class (donor or acceptor), $a^* = 21 \times 10^{-8}$ cm is the effective Bohr radius, $\alpha = 3.6 \times 10^{-8}$ eV cm, and 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 <u>ZEROIN</u> [11-13] which searches for a zero of the parameter TEST. <u>ZEROIN</u> 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, <u>ZEROIN</u> 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 stopping criterion is $\left| \frac{\text{EF}-\text{EFG}}{2} \right| \leq \text{RE } \times \text{EF} + \text{AE} ,$

where RE is the maximum allowable relative error and AE is the maximum allowable absolute error in eV. In the calling program these are both assigned the value 1 x 10^{-6} so that they have equal weight in the stopping criterion when EF = 1.0 eV. Initially, the subroutine compares RE 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 TEST(EF) < TEST(EFG) . 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 TEST(EF) = 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 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 al.* [14], and the magnitude is based on the results at 300 K of Thurber *et al.* [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 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

Mathematical Symbol	Program Name	Definition*
ND	SUMTD	Total donor density (cm ⁻³)
NA	SUMTA	Total acceptor density (cm ⁻³)
μL	ULN ULP	Lattice mobility for electrons (cm ² /V·s) Lattice mobility for holes (cm ² /V·s)
μI	UIN UIP	Ionized impurity mobility for electrons (cm ² /V·s) Ionized impurity mobility for holes (cm ² /V·s)
Ŷ	GAMMA	Factor giving effect of carrier-carrier scattering on ionized impurity mobility
NI	CION	Density of ionized impurities (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
N _D +	SUMID	Total ionized donor density (cm ⁻³)
N _A +	SUMIA	Total ionized acceptor density (cm ⁻³)
n'	CNSTAR	Effective electron screening density (cm ⁻³)
p '	CPSTAR	Effective hole screening density (cm ⁻³)
4πκεο	DIEL	4π times relative dielectric constant times permittivity of free space
k		Boltzmann constant
h		Planck constant ($\hbar = h/2\pi$)
q		Electronic charge
m _o		Free electron mass
		Longitudinal effective mass (in units of $m_{ m O}^{})$
^m d [*]		Density-of-states effective mass (in units of $m_{0}^{}$)
m_*		Conductivity effective mass (in units of $m_{ m o}^{}$)
μN	UNIS	Neutral impurity scattering mobility $(cm^2/V \cdot s)$
NN	CNUT	Density of neutral impurities (cm ⁻³)
n	CN	Electron density (cm ⁻³)
р	СР	Hole density (cm ⁻³)

Table 1. Symbols Used in Mobility Formulas.

* Quantities in SI units unless otherwise stated.

Scattering Mechanism	Formula	Statement Number*
Lattice + electron-electron	$\begin{split} & N_D < 3 \times 10^{17} \ \text{cm}^{-3} \\ & T \leq 108 \ \text{K} \mu_L = 1.89 \times 10^7 \text{T}^{-1} \cdot 52 \ [1 - 0.08 \ \text{N}_D / (2 \times 10^{17})] \\ & T > 108 \ \text{K} \mu_L = 7.98 \times 10^8 \text{T}^{-2} \cdot 32 \ [1 - 0.08 \ \text{N}_D / (2 \times 10^{17})] \\ & N_D \geq 3 \times 10^{17} \ \text{cm}^{-3} \end{split}$	8 10
	$T \le 108 \text{ K} \ \mu_L = 1.89 \times 10^7 \text{T}^{-1.52} \ (0.884)$ $T > 108 \text{ K} \ \mu_L = 7.98 \times 10^8 \text{T}^{-2.32} \ (0.884)$	22 30
Ionized impurity + electron-electron	$\mu_{I} = \gamma \times 7.3 \times 10^{17} T^{1.5} / N_{I}G(b)$ $\mu_{I} = \frac{N_{D}^{+}}{10^{10}} [1 - \alpha_{N} p(-p_{1}^{+}/N_{0}^{+}+)]$	90
	$\gamma = \frac{1}{n'} [1 - exp(-n/N_D^*)]$ $n' = n + p + N_D^+ (1 - N_D^+/N_D)$ $G(b) = \ln(b + 1) - b/(b + 1)$ $b = \frac{24\kappa}{q^2\hbar^2n'} \times 10^{-6}$	80 42 80 52
Combined lattice and ionized im- purity	$\mu_{\text{LI}} = \mu_{\text{L}} f(X)$ $f(X) = 1 + X^{2} [CiXcosX + sinX(SiX - \frac{\pi}{2})]$ $X^{2} = 6 \mu_{\text{L}}/\mu_{\text{I}}$	104 104 98
Neutral impurity	$\mu_{N} = 0.82 \ \mu_{E} \ \left[\frac{2}{3} \ \left(\frac{kT}{E_{N}}\right)^{1/2} + \frac{1}{3} \ \left(\frac{E_{N}}{kT}\right)^{1/2}\right]$ $E_{N} = \frac{1.136 \times 10^{-19} \ m_{d}^{\star}}{\kappa^{2} \ m_{o}}$ $\mu_{E} = \frac{2\pi^{3}q^{3} \ m_{d}^{\star}}{5N_{N} \ 4\pi\kappa \varepsilon_{o} \ h^{3}} \times 10^{-2}$	114 112 110
Total electron mobility	$\mu = (1/\mu_{LI} + 1/\mu_{N})^{-1}$	116

Table 2. Formulas for Calculating Electron Mobility.

*These statement numbers refer to subroutine MOB.

Scattering Mechanism	Formula	Statement Number*
Lattice +	$N_{\rm A} < 3 \times 10^{17} \rm \ cm^{-3}$	
hole-hole	T < 72 K μ_{L} = 1.6 × 10 ⁷ T ^{-1.54} [1 - 0.08 N _A /(2 × 10 ¹⁷)]	118
	$T \ge 72 \text{ K}$ $\mu_{L} = 2.3 \times 10^{9} \text{ T}^{-2.7} [1 - 0.08 \text{ N}_{\text{A}}/(2 \times 10^{17})]$	120
	$N_A \ge 3 \times 10^{17} \text{ cm}^{-3}$	
	$T < 72 \text{ K} \mu_{L} = 1.6 \times 10^{7} \text{T}^{-1} \cdot 54$ (0.884)	132
	$T \ge 72 \text{ K} \ \mu_{L} = 2.3 \times 10^{9} \text{T}^{-2.7} (0.884)$	140
Ionized impurity	$\mu = \frac{\gamma [\mu_{11} + \mu_{12} (m_{d2}^{*}/m_{d1}^{*})^{1.5} + \mu_{13} (m_{d3}^{*}/m_{d1}^{*})^{1.5} \exp(-0.044/kT)]}{(m_{d3}^{*}/m_{d1}^{*})^{1.5} \exp(-0.044/kT)]}$]
1016-1016	$\prod_{M^+} [1 + (m_{d3}^*/m_{d1}^*)^{1.5} + (m_{d3}^*/m_{d1}^*)^{1.5} \exp(-0.044/kT)]$	150
	$\gamma = \frac{N_A}{p'} [1 - exp(-p'/N_A^+)]$	198
	$p' = p + n + N_A^+ (1 - N_A^+/N_A)$	152
	for i = 1, 2, 3	
	$\mu_{Ii} = \frac{2^{3 \cdot 5} (4\pi \kappa \epsilon_0)^2 \hat{m_{di}^{0.5}(kT)^{1.5}}}{\pi^{1.5} q^3 m_{ci}^{\star} N_I G(b_i)} \times 10^{-2}$	192
	$G(b_i) = ln(b_i + 1) - b_i/(b_i + 1)$	190
	b. = $\frac{24\kappa\epsilon_0 m_{di}^{*} (kT)^2}{10^{-6}} \times 10^{-6}$	162
	¹ q ² ħ ² p'	
Combined lattice	$\mu_{LI} = \mu_{L} f(X)$	214
purity	$f(X) = 1 + X^2 [CiXcosX + sinX(SiX - \frac{\pi}{2})]$	214
	$X^2 = 6 \mu_L / \mu_I$	208
Neutral impurity	$[\mu_{N]} + \mu_{N2} (m_{d2}^{*}/m_{d1}^{*})^{1.5} + \mu_{N3} (m_{d3}^{*}/m_{d1}^{*})^{1.5} \exp(-0.044/kT)]$	
	$\mu_{N} = \frac{1}{[1 + (m_{d2}^{*}/m_{d1}^{*})^{1.5} + (m_{d3}^{*}/m_{d1}^{*})^{1.5} \exp(-0.044/kT)]}$	224
	for $i = 1, 2, 3$ $1/2$ $= 1/2$	
	$\mu_{Ni} = 0.82 \ \mu_{Ei} \left[\frac{2}{3} \left(\frac{kT}{E_{Ni}}\right) + \frac{1}{3} \left(\frac{CNi}{kT}\right)\right]$	222
	$E_{Ni} = \frac{1.136 \times 10^{-19} \text{ m}_{di}^{*}}{\kappa^2 \text{ m}_{o}}$	221
	$\mu_{\text{Ei}} = \frac{2\pi^3 q^3 m_{di}^*}{5N_N 4\pi \kappa \varepsilon_0 h^3} \times 10^{-2}$	220
Total hole mobility	$\mu = (1/\mu_{LI} + 1/\mu_{N})^{-1}$	226

Table 3. Formulas for Calculating Hole Mobility.

* These statement numbers refer to subroutine $\underline{\text{MOB}}$.

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 relative 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 = $(1.2711 \times 10^{-9}) \exp(7.8 \times 10^{-5} \text{T})$ 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	DIZ
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
EG = THE ENERGY GAP OF SILICON IN ELECTRON VOLTS
       EXCITON ENERGY OF 0.01 EV IS NOT INCLUDED IN EG
EF = FERMI LEVEL IN EV (DETERMINED IN PROGRAM BY TRIAL AND ERROR)
       EF IS TAKEN TO BE ZERO AT THE VALENCE BAND EDGE
CN = THE CONCENTRATION OF ELECTRONS IN THE CONDUCTION BAND IN CM-3
CP = 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.

С

```
С
              'DOUBLE OFF' RESTORES SINGLE OUTPUT LINE FORMAT
              "CONSTANTS" GENERATES A PAGE OF THE PARAMETERS THAT DO NOT
С
С
                     CHANGE WITH DOPING LEVEL
С
              "DOLOOP XX" (WHERE XX = D1 - A3) PRODUCES MULTIPLE RUNS
С
                     CARD FORMAT = DOLOOP XX, INC. DENSITY, NO. OF RUNS
С
              'STOP' IS USED TO TERMINATE THE SESSION WITH THE COMPUTER
С
      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=1.6022E-19
      INITIALIZE THE SETTINGS OF THE OPTION SWITCHES
С
      LOOPSW=0.
      DOUBSW=6H0FF
С
С
      READ THE D1 DATA (OR CONTROL) CARD
10
      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
С
С
      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
20
      FORMAT (2A6, E10.4, 2F10.4)
С
      IF (LOOPSW.EQ.O.) GO TO 50
С
      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
30
      PRINT 40
40
      FORMAT (1H0,26HLOOPSWITCH IS OUT OF RANGE)
      GO TO 10
С
      RUNNO=1. DURING FIRST RUN, THEN 2. UP TO 77 KELVIN, THEN 3. TO
С
              ROOM TEMPERATURE, THEN 4. ABOVE ROOM TEMPERATURE
50
      RUNNO=1.
```

```
С
      CALULATE REDUCTION IN ACTIVATION ENERGIES
      EQUATION OF PENIN ET AL. FOR PHOSPHORUS-DOPED SILICON IS
С
С
             GENERALIZED FOR USE WITH OTHER ACTIVATION ENERGIES
С
             SEE PAPER IN SOVIET PHYS.-SOLID STATE 7, 2580 (1966)
      SUMTD=DN1+DN2
С
     GUARD AGAINST ZERO DIVISOR IN CALCULATION OF RDD
     IF (SUMTD.LE.O.) RDD=1.E20
      IF (SUMTD.LE.O.) GO TO 60
     RDD=1.E8*(3./(4.*3.1416*SUMTD))**0.3333
60
      SUMTA=DN3+DN4+DN5
      GUARD AGAINST ZERO DIVISOR IN CALCULATION OF RDA
С
      IF (SUMTA.LE.O.) RDA=1.E20
      IF (SUMTA.LE.O.) GO TO 70
      RDA=1.E8*(3./(4.*3.1416*SUMTA))**0.3333
70
      EN1=ENIN1
С
      FOLLOWING STATEMENT COMPUTES THE REDUCTION IN ACTIVATION ENERGY
С
             OMIT THIS STATEMENT IF FIXED ENERGY LEVEL ENIN1 IS DESIRED
С
             SAME COMMENTS APPLY TO OTHER DOPANT STATES
     EN1=ENIN1-0.36*(0.5+21./RDD)*EXP(-RDD/21.)-3.6E-8*SUMTA**0.3333
     IF (EN1-0.0) 80,90,90
С
      IF ANY ACTIVATION ENERGY IS NEGATIVE, SET IT EQUAL TO ZERO
80
     EN1=0.0
90
      EN2=ENIN2
     EN2=ENIN2-0.36*(0.5+21./RDD)*EXP(-RDD/21.)-3.6E-8*SUMTA**0.3333
     IF (EN2-0.0) 100,110,110
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*(U.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
     EN5=0.0
     THE FIRST TEMPERATURE WILL BE 4.2 KELVIN
С
170
     T=4.2
С
     T WILL BE INCREMENTED IN EQUAL 1000/T INTERVALS
      RTEMP=1000./T
С
С
      SET UP THE OUTPUT PAGE
     WRITE (6,180)
      FORMAT (1H1, 32HELECTRICAL PROPERTIES OF SILICON)
180
      IF (NAME1(1).EQ.6HCONSTA) GO TO 320
      READ-OUT ALL PERTINENT INPUT DATA
С
      WRITE (6,190)
190
      FORMAT (1H0,26HD0PANT STATES FOR THIS RUN)
      WRITE (6,200)
                                                                       Е
                                        DENSITY
                                                     ENERGY(INPUT)
200
     FORMAT (1HO,77H
                        DOPANT
     2NERGY(CALC.) DEGENERACY)
```

```
IF (NAME1(1).EQ.6HDUMMY ) GO TO 210
      WRITE (6,250) NAME1, DN1, ENIN1, EN1, DG1
      IF (NAME2(1).EQ.6HDUMMY ) GO TO 220
210
      WRITE (6,250) NAME2, DN2, ENIN2, EN2, DG2
220
      IF (NAME3(1).EQ.6HDUMMY ) GO TO 230
      WRITE (6,250) NAME3, DN3, ENIN3, EN3, DG3
      IF (NAME4(1).EQ.6HDUMMY ) GO TO 240
230
      WRITE (6,250) NAME4, DN4, ENIN4, EN4, DG4
240
      IF (NAME5(1).EQ.6HDUMMY ) GO TO 260
      WRITE (6,250) NAME5, DN5, ENIN5, EN5, DG5
      FORMAT (1X, 2A6, 6X, 1PE9.3, 7X, 0PF7.4, 8X, F8.4, 10X, F8.4)
250
260
      WRITE (6,270)
270
      FORMAT (1HO)
С
      PROVIDE COLUMN HEADINGS FOR OUTPUT TABLE
      WRITE (6,280)
280
      FORMAT (1HO, 129H
                         TEMP
                                     1000/T
                                                 EF
                                                             N
                                                                         Ρ
             COND. MOB
                                                D1 ION
                                                           DZ ION
     2
                           RH
                                       RHO
                                                                       A1
     3ION
            A2 ION)
      WRITE (6,290)
      FORMAT (1H )
290
      IF (DOUBSW.NE.6HON ) GO TO 350
      WRITE (6,300)
300
      FORMAT (1H ,130H
                          EG
                                     TEST
                                                KT/Q
                                                            EG-EF
                                                                       A3
                       MOB-(LAT) +IONIZED
                                               +NEUTRAL MOB+(LAT)
     2ION
               SIGMA
                                                                     +IONI
     3ZED
            +NEUTRAL)
      WRITE (6,310)
310
      FORMAT (1HO)
      GO TO 350
С
      COLUMN HEADINGS FOR 'CONSTANTS' OPTION
320
      WRITE (6,330)
     FORMAT (1HO,128H
330
                         TEMP
                                    1000/T
                                                KT/Q
                                                             EG
                                                                        DI
     2EL
           MOB-(LAT)
                       MOB+(LAT) T**3/2
                                                  ME
                                                             MH
                                                                        FN
     30
               FNV)
      WRITE (6,340)
340
      FORMAT (1HO)
С
      EFME AND EFMH ARE THE EFFECTIVE MASSES OF ELECTRONS AND HOLES
С
      1039 (1967). EFME AND EFMH EQS FITTED OVER TEMP RANGE O TO 600 K
350
      EFME=((((((4.54649E-17*T-9.66067E-14)*T+8.04032E-11)*T-3.320130E-8)
     2*T+6.83008E-6)*T-.000161708)*T+1.0627
352
      EFMH=((((((1.11997E-16*T-2.596730E-13)*T+2.30049E-10)*T-9.67212E-8)
     2*T+1.85678E-5)*T-.000523548)*T+.590525
353
      CAYT=8.6173E-5*T
С
      CONST = 2*(2*PI*K*(FREE ELECTRON MASS)/H**2)**(3/2)
      CONST=4.829E15
      TPOWR=T**1.5
С
      FNC AND FNV ARE THE DENSITY OF STATES IN THE CONDUCTION AND
С
             VALENCE BANDS RESPECTIVELY
354
      FNC=CONST*(EFME**1.5)*TPOWR
355
      FNV=CONST*(EFMH**1.5)*TPOWR
      EG FROM FIT OF DATA FROM MACFARLANE, PHYS. REV. 111, 1245 (1958)
С
356
      EG=(((-3.80977E-13*T+9.95E-10)*T-8.70110E-7)*T+.0000323741)*T+1.15
     2556
С
      IN 'CONSTANTS' OPTION, WE NEED NOT DETERMINE EF
```

```
IF (NAME1(1).EQ.6HCONSTA) GO TO 530
      EF=0.0
      EFG=1.2
      RE=1.0E-6
      AE=1.0E-6
      IFLAG=0
С
      CALL SUBROUTINE TO FIND VALUE OF EF WHICH MAKES TEST VERY SMALL
      CALL ZEROIN (TEST, EF, EFG, RE, AE, IFLAG)
      IF (IFLAG.GT.2) GO TO 690
С
С
      CALL SUBROUTINE TO CALCULATE MOBILITY
      CALL MOB
С
      ERROR AND/OR WARNING DIAGNOSTIC MESSAGES
      IF (ALPHA.LT.-2.) GO TO 370
      WRITE (6,360) ALPHA
360
     FORMAT (20X, 15H(EF-EG)/CAYT = ,F8.4,
     2 33H ERROR IN N MAY EXCEED 1 PERCENT)
370
     IF (BETA.LT.-2.) GO TO 390
      BETAN=-BETA
      WRITE (6,380) BETAN
     FORMAT (20X, 10HEF/CAYT = , F8.4,
380
    2 33H ERROR IN P MAY EXCEED 1 PERCENT)
390
    IF (ISTAT.GE.10000) WRITE (6,400)
400
     FORMAT (20x,72HBORN APPROXIMATION FOR IONIZED SCATTERING NOT VALID
     2 FOR MAJORITY CARRIER)
С
С
      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.9.999999919.AND.RH.NE.O.) WRITE (6,450) RH
      IF (RH.NE.9.999999919.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
     FORMAT (1H+,33X,1PE11.3)
420
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)
      FORMAT (1H+,121X,1PE10.3)
500
      IF (DOUBSW.NE.6HON ) GO TO 590
      OUT3=EG-EF
      TESTF=TEST(EF)
      WRITE (6,510) EG, TESTF, CAYT, OUT3
      FORMAT (F11.6, 1PE11.3, 1PE11.4, 2X, F9.6)
510
      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.O.) WRITE (6,500) UDP
      WRITE (6,520)
     FORMAT (1HO)
520
     GO TO 590
     OUTPUT INSTRUCTIONS FOR THE 'CONSTANTS' OPTION
С
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
    ULN=7.98E8*T**(-2.32)
540
550 IF (T.GE.72.) GO TO 560
     ULP=1.6E7*T**(-1.54)
     GO TO 570
560
    ULP=2.3E9*T**(-2.7)
570
     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)
С
     SET UP NEXT TEMPERATURE
     THE MAXIMUM TEMPERATURE OF INTEREST IS 500 DEGREES KELVIN
С
590 IF (T-500.) 600,710,710
600 IF (RUNNO-2.) 610,620,630
610
     RUNNO=2.
С
      SECOND TIME AROUND, THE TEMPERATURE WILL BE 20 DEGREES KELVIN
      T=20.
      RTEMP=1000./T
      GO TO 350
С
     AFTER THE SECOND TIME AROUND, 1000./T IS DECREMENTED BY 2.
620
     RTEMP=RTEMP-2.
      T=1000./RTEMP
     AN EVALUATION AT LIQUID NITROGEN TEMPERATURE IS DESIRED
С
      IF (T.GE.77.) GO TO 640
      GO TO 350
      IF (T.EQ.77.) GO TO 650
630
      AN EVALUATION AT ROOM TEMPERATURE (300 KELVIN) IS DESIRED
С
      IF (RUNNO.EQ.4.) GO TO 680
      IF (T.EQ.300.) GO TO 670
С
      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./T
      RUNNO=3.
     GO TO 350
650
     RTEMP=12.
      T=1000./RTEMP
```

	GO TO 350
660	T=300.
	RTEMP=1000./T
	GO TO 350
670	RTEMP=3.
	T=1000./RTEMP
	RUNNO=4.
	GO TO 350
С	ABOVE ROOM TEMPERATURE 1000./T IS DECREMENTED BY 0.5
680	RTEMP=RTEMP-0.5
	T=1000./RTEMP
	GO TO 350
690	WRITE (6,700) IFLAG
700	FORMAT (1H0,51HCHARGE BALANCE EQUATION COULD NOT BE SOLVED, IFLAG=
	2,11)
	GO TO 590
710	IF (DOUBSW.NE.6HON) GO TO 720
С	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
С	ROUTINE TO SET-UP OR CANCEL DOUBLE OUTPUT LINE FORMAT
С	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
С	DEFAULT VALUE IS TAKEN TO MEAN 'DOUBLE OFF'
	DOUBSW=6HOFF
	GO TO 10
С	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	FORMAT (1HO, 34HINVALID ARGUMENT OF DOLOOP COMMAND)
7/5	GO TO TU
760	STOP
	END

FUNCTION TEST (EF)

С С THIS EXTERNAL FUNCTION DEFINES THE PARAMETER 'TEST'. С 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 С С COMPUTATION OF CN 2 CN=O. 4 ALPHA=(EF-EG)/CAYT IF (ALPHA.GT.1.) GO TO 10 IF (ALPHA.LE.-80.) GO TO 20 С THE FOLLOWING EQUATION IS USED FOR ALPHA BETWEEN -80 AND +1 8 CN=FNC/((EXP(-ALPHA))+0.27) GO TO 20 С THE FOLLOWING EQUATION IS USED FOR ALPHA GREATER THAN +1 10 CN=FNC*0.752253*((ALPHA*ALPHA+1.7)**0.75) COMPUTATION OF CP С 20 CP=0. 22 BETA=-EF/CAYT IF (BETA.GT.1.) GO TO 30 IF (BETA.LE.-80.) GO TO 40 С THE FOLLOWING EQUATION IS USED FOR BETA BETWEEN -80 AND +1 26 CP=FNV/((EXP(-BETA))+0.27) GO TO 40 С THE FOLLOWING EQUATION IS USED FOR BETA GREATER THAN +1 30 CP=FNV*0.752253*((BETA*BETA+1.7)**0.75) COMPUTATION OF DI1 С 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 С 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 DI2=DN2/(1.+(EXP(POWER)*DG2)) GO TO 80 70 DI2=DN2 С

COMPUTATION OF DI3

80 DI3=0. IF (NAME3(1).EQ.6HDUMMY) GO TO 100 POWER=(EN3-EF)/CAYT IF (POWER.GE.80.) GO TO 100 IF (POWER.LE. -80.) GO TO 90 DI3=DN3/(1.+(EXP(POWER)*DG3)) GO TO 100 90 DI3=DN3 С COMPUTATION OF DI4 100 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 COMPUTATION OF DI5 С 120 DI5=0. IF (NAME5(1).EQ.6HDUMMY) 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 140 130 DI5=DN5 TESTING TO SEE HOW CLOSE TO NEUTRALITY WE HAVE COME С THE PARAMETER TEST IS THE NET DENSITY OF RESIDUAL CHARGES С С WHEN THE FERMI LEVEL IS AT ITS PRESENT POSITION 140 TEST=(CN+DI3+DI4+DI5)-(CP+DI1+DI2)RETURN END

SUBROUTINE ZEROIN(F,B,C,RE,AE,IFLAG) С С SANDIA MATHEMATICAL PROGRAM LIBRARY С MATHEMATICAL COMPUTING SERVICES DIVISION 5422 С SANDIA LABORATORIES С P. O. BOX 5800 С ALBUQUERQUE, NEW MEXICO 87115 С CONTROL DATA 6600 VERSION 4.5, 1 NOVEMBER 1971 С С MODIFIED TO RUN AT NBS BY D. KAHANER DIV 713 С С ABSTRACT С ZEROIN SEARCHES FOR A ZERO OF A FUNCTION F(X) BETWEEN С THE GIVEN VALUES B AND C UNTIL THE WIDTH OF THE INTERVAL С (B,C) HAS COLLAPSED TO WITHIN A TOLERANCE SPECIFIED BY С THE STOPPING CRITERION, ABS(B-C) .LE. 2.*(RW*ABS(B)+AE). С С DESCRIPTION OF ARGUMENTS С - NAME OF THE REAL VALUED EXTERNAL FUNCTION. THIS NAME F С MUST BE IN AN EXTERNAL STATEMENT IN THE CALLING С PROGRAM. F MUST BE A FUNCTION OF ONE REAL ARGUMENT. С В - ONE END OF THE INTERVAL (B,C). THE VALUE RETURNED FOR С B USUALLY IS THE BETTER APPROXIMATION TO A ZERO OF F. С - THE OTHER END OF THE INTERVAL (B,C) С С RE - RELATIVE ERROR USED FOR RW IN THE STOPPING CRITERION. С IF THE REQUESTED RE IS LESS THAN MACHINE PRECISION, С THEN RW IS SET TO APPROXIMATELY MACHINE PRECISION. С - ABSOLUTE ERROR USED IN THE STOPPING CRITERION. IF THE AE С GIVEN INTERVAL (B,C) CONTAINS THE ORIGIN, THEN A С NONZERO VALUE SHOULD BE CHOSEN FOR AE. С IFLAG - RETURNS A STATUS OF THE RESULTS INDICATING WHICH С OF THE FOLLOWING CONDITIONS HOLD. С A - ABS(B-C) .LE. 2.*(RW*ABS(B)+AE) С B - F(B) * F(C) .LT. 0.С C - ABS(F(B)) .LE. ABS(F(C)) С D - ABS(F(B)) .LE. MAX(ABS(F(B)), ABS(F(C))) С OUT IN IN С E - NUMBER OF EVALUATIONS OF F(X) .LE. 500 С =1 INDICATES NORMAL CASE. ALL CONDITIONS ABOVE HOLD. C =2 INDICATES F(B) = 0. CONDITION A MAY NOT HOLD. С =3 INDICATES CONDITIONS A, B, C, AND E HOLD BUT D DOES С NOT. (B,C) PROBABLY CONTAINS A SINGULAR POINT OF F. С =4 INDICATES CONDITIONS A AND E HOLD BUT B DOES NOT. С A LOCAL MINIMUM OF F(X) IN (B,C) MAY HAVE BEEN FOUND. С =5 INDICATES SEARCH WAS ABORTED WHEN CONDITION E FAILED. С С REFERENCES С 1. L F SHAMPINE AND H A WATTS, ZEROIN, A ROOT-SOLVING CODE, С SC-TM-70-631, SEPT 1970. С 2. T J DEKKER, FINDING A ZERO BY MEANS OF SUCCESSIVE LINEAR С INTERPOLATION, *CONSTRUCTIVE ASPECTS OF THE FUNDAMENTAL С THEOREM OF ALGEBRA*, EDITED BY B DEJON AND P HENRICI, 1969. С

3. L F SHAMPINE AND R C ALLEN, NUMERICAL COMPUTING--

```
С
             AN INTRODUCTION, 1973.
С
С
      INITIALIZE FOR UNIVAC 1108
      DATA ER/6.0E-8/
С
      INITIALIZE IN PORTABLE MANNER
С
      DATA ER/0.0/
С
      IF (ER .EQ. 0.0) ER = 4 + (R1MACH (4))
С
      RW=AMAX1(RE,ER)
      IC=0
      ACBS=ABS(B-C)
      A = C
      FA = F(A)
      FB=F(B)
      FC=FA
      KOUNT=2
      FX=AMAX1(ABS(FB),ABS(FC))
С
    1 IF (ABS(FC) .GE. ABS(FB)) GO TO 2
С
      PERFORM INTERCHANGE
      A=B
      FA=FB
      B=C
      FB=FC
      C = A
      FC=FA
С
    2 CMB=0.5*(C-B)
      ACMB=ABS(CMB)
      TOL=RW*ABS(B)+AE
С
С
      TEST STOPPING CRITERION
      IF (ACMB .LE. TOL) GO TO 10
С
С
      CALCULATE NEW ITERATE IMPLICITLY AS B+P/Q
С
      WHERE WE ARRANGE P .GE. O.
С
      THE IMPLICIT FORM IS USED TO PREVENT OVERFLOW.
      P=(B-A)*FB
      Q=FA-FB
      IF (P .GE. 0.) GO TO 3
      P = -P
      Q = -Q
С
      UPDATE A AND CHECK FOR SATISFACTORY REDUCTION
С
С
      IN THE SIZE OF OUR BOUNDING INTERVAL.
    3 A=B
      FA=FB
      IC=IC+1
      IF (IC .LT. 4) GO TO 4
      IF (8.*ACMB .GE. ACBS) GO TO 6
      IC=0
      ACBS=ACMB
```

```
С
```

```
TEST FOR TOO SMALL A CHANGE
С
    4 IF (P .GT. ABS(Q)*TOL) GO TO 5
С
С
      INCREMENT BY TOLERANCE
      B=B+SIGN(TOL,CMB)
      GO TO 7
С
     ROOT OUGHT TO BE BETWEEN B AND (C+B)/2.
С
    5 IF (P .GE. CMB*Q) GO TO 6
С
С
      INTERPOLATE
      B=B+P/Q
      GO TO 7
С
    6 B=0.5*(C+B)
С
      BISECT
С
С
      HAVE COMPLETED COMPUTATION FOR NEW ITERATE B
    7 FB=F(B)
      IF (FB .EQ. 0.) GO TO 11
      KOUNT=KOUNT+1
      IF (KOUNT .GT. 500) GO TO 15
С
С
      DECIDE WHETHER NEXT STEP IS INTERPOLATION OR EXTRAPOLATION
      IF (SIGN(1.0,FB) .NE. SIGN(1.0,FC)) GO TO 1
      C=A
      FC=FA
      GO TO 1
С
С
С
      FINISHED. PROCESS RESULTS FOR PROPER SETTING OF IFLAG
С
   10 IF (FB*FC .GT. 0.) GO TO 13
      IF (ABS(FB) .GT. FX) GO TO 12
      IFLAG = 1
      RETURN
   11 IFLAG = 2
      RETURN
   12 \text{ IFLAG} = 3
      RETURN
   13 \text{ IFLAG} = 4
      RETURN
   15 \text{ IFLAG} = 5
      RETURN
      END
```

SUBROUTINE MOB

С С

С

С С

С

С С

С

С

С

2

С С

С

С

С

С

С

С

С

С

8

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*PI*(ABSOLUTE 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=DI3+DI4+DI5 CION=DI1+DI2+DI3+DI4+DI5 CNUT=DN1+DN2+DN3+DN4+DN5-CION 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 ELECTRON 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=1.89E7*T**(-1.52)*(1.-0.08*SUMTD/2.E17) GO TO 40 ULN=7.98E8*T**(-2.32)*(1.-0.08*SUMTD/2.E17) 10 GO TO 40 20 IF (T.GE.108.) GO TO 30 22 ULN=1.89E7*(T**(-1.52))*0.884 GO TO 40 30 ULN=7.98E8*(T**(-2.32))*0.884 ADD ON THE EFFECTS OF IONIZED IMPURITY SCATTERING С WE MUST ALLOW FOR THE FACT THAT SUMTD MIGHT VANISH IN CNSTAR EQ. С 40 IF (SUMTD.LE.O.) CNSTAR=CN+CP IF (SUMTD.LE.O.) GO TO 50

```
42
      CNSTAR=CN+CP+(1.-SUMID/SUMTD)*SUMID
С
      BN IS LOG TERM IN MODIFIED BROOKS-HERRING IONIZED IMPURITY MOB. EQ
С
      BN = 6*DIEL*MASS*(1.3806E-23)**2*T*T/(PI*Q*Q*HBAR*HBAR*CNSTAR)
С
      WE MUST ALLOW FOR THE FACT THAT CNSTAR MIGHT VANISH IN EQ FOR BN
С
             BN IS SET TO A LARGE NUMBER AND FIRST POSITION OF ISTAT
С
             IS SET TO UNITY
50
      IF (CNSTAR.LE.O.) BN=9.999999E19
      IF (CNSTAR.LE.O.) ISTAT=ISTAT+1
      IF (CNSTAR.LE.O.) GO TO 80
52
      BN=1.14E24*DIEL*T*T/CNSTAR
С
      IF BN IS SMALL, BORN APPROXIMATION IS NOT VALID. IN THIS CASE,
             FIFTH POSITION OF ISTAT IS INCREMENTED.
С
      IF (BN-10.) 60,60,80
60
      ISTAT=ISTAT+10000
      IF (CION-1.0) 70,80,80
70
      UDN=ULN
      OUT8=UDN
      GO TO 110
08
      GN=ALOG(BN+1.)-BN/(BN+1.)
С
      CALCULATE GAMMA FOR EFFECT OF E-E SCATTERING ON ION. IMP. MOBILITY
      IF (CNSTAR.LE.O.) GAMMA=0.632
      IF (CNSTAR.LE.O.) GO TO 90
      IF (SUMID.LE.O.) GAMMA=0.432
86
      IF (SUMID.GT.O.) GAMMA=(SUMID/CNSTAR)*(1.-EXP(-CNSTAR/SUMID))
      IF (GAMMA.LT.0.432) GAMMA=0.432
      UIN=GAMMA*7.3E17*TPOWR/(CION*GN)
90
      IF (UIN.LE.O.) RATION=1.E6
      IF (UIN.LE.O.) GO TO 100
98
      RATION=6.*ULN/UIN
100
     XN=SQRT(RATION)
      COMBINE LATTICE AND IONIZED IMPURITY SCATTERING BY THE MIXED-
С
С
             SCATTERING FORMULA OF DEBYE AND CONWELL, PHYS. REV. 93,
С
             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)))
104
      OUT8=UDN
С
      ADD ON THE EFFECTS OF NEUTRAL IMPURITY SCATTERING
С
      NEUTRAL IMPURITY MOBILITY AS PER ERGINSOY, PHYS REV 79,1013 (1950)
С
      UNIS = 0.02*PI**3*Q**3*MASS/(5*DIEL*CNUT*H**3)
С
      UNIS CONTAINS GEOMETRIC MEAN MASS WITH VALUE OF EFME/6**0.667
С
      SEE BROOKS, ADV. IN ELECTRONICS AND ELECTRON PHYSICS 7, 161 (1955)
110
      UNIS=4.85E11*EFME/(DIEL*CNUT)
С
      SCLAR'S CORRECTION TO UNIS, SEE PHYS REV 104, 1559 (1956)
С
      SEE ALSO PAPER BY LI AND THURBER, SSE 20, 609 (1977)
112
      EI=0.215*EFME/((DIEL/1.1121E→10)**2*CAYT)
114
      UNIS=UNIS*0.82*(2*SQRT(1/EI)/3+SQRT(EI)/3.)
116
     UDN=1/(1/UDN+1/UNIS)
С
      THAT COMPLETES THE COMPUTATION OF THE ELECTRON MOBILITY
С
      CALCULATION OF HOLE MOBILITY
С
      LATTICE SCATTERING WITH CORRECTION FOR HOLE-HOLE SCATTERING
С
      EQ FOR ULP FOR T.LT.72 FROM BRAGGINS, PHD THESIS,
С
             SYRACUSE UNIVERSITY, 1975
С
     EQ FOR ULP FOR T.GE.72 FROM LUDWIG AND WATTERS,
```

```
С
             PHYS REV 101, 1699 (1956)
      IF (SUMTA.GE.3.E17) GO TO 130
      IF (T.GE.72.) GO TO 120
      ULP=1.6E7*T**(-1.54)*(1.-0.08*SUMTA/2.E17)
118
      GO TO 150
      ULP=2.3E9*T**(-2.7)*(1.-0.08*SUMTA/2.E17)
120
      GO TO 150
130
      IF (T.GE.72.) GO TO 140
      ULP=1.6E7*(T**(-1.54))*0.884
132
      GO TO 150
140
      ULP=2.3E9*(T**(-2.7))*0.884
      ADD ON THE EFFECTS OF IONIZED IMPURITY SCATTERING
C
      WE MUST ALLOW FOR THE FACT THAT SUMTA MIGHT VANISH IN CPSTAR EQ.
С
150
      IF (SUMTA.LE.O.) CPSTAR=CN+CP
      IF (SUMTA.LE.O.) GO TO 160
      CPSTAR=CP+CN+(1.-SUMIA/SUMTA)*SUMIA
152
С
      BP IS LOG TERM IN BROOKS-HERRING IONIZED IMPURITY MOBILITY
С
      BP = 6*DIEL*MASS*(1.3806E-23)**2*T*T/(PI*Q*Q*HBAR*HBAR*CPSTAR)
С
      MASS FOR BP OF EACH BAND FROM LI, NBS SPECIAL PUBLICATION 400-47
С
      NO TEMPERATURE DEPENDENCE FOR MASS, 300 K VALUE USED
С
             IS SET TO 1
      WE MUST ALLOW FOR THE FACT THAT CPSTAR MIGHT VANISH IN EQ FOR BP
С
С
             BP IS SET TO A LARGE NUMBER AND THIRD POSITION OF ISTAT
      IF (CPSTAR.LE.O.) BP1=9.999999E19
160
      IF (CPSTAR.LE.O.) BP2=9.999999E19
      IF (CPSTAR.LE.O.) BP3=9.999999E19
      IF (CPSTAR.LE.O.) ISTAT=ISTAT+100
      IF (CPSTAR.LE.O.) GO TO 190
      BP1=1.16E24*0.568*DIEL*T*T/CPSTAR
162
      BP2=1.16E24*0.412*DIEL*T*T/CPSTAR
      BP3=1.16E24*0.246*DIEL*T*T/CPSTAR
      IF BP IS SMALL, BORN APPROXIMATION IS NOT VALID. IN THIS CASE,
С
             FIFTH POSITION OF ISTAT IS INCREMENTED.
С
      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.)
      GP2=ALOG(BP2+1.)-BP2/(BP2+1.)
      GP3=ALOG(BP3+1.)-BP3/(BP3+1.)
      UIP = 0.01*(2**3.5)*DIEL*DIEL*SQRT(MD)*(1.38E-23*T)**1.5/
С
             ((PI**1.5)*Q*Q*Q*MC*CION*GP)
С
      UIP1=2.66E35*DIEL*DIEL*TPOWR*SQRT(0.568)/(0.448*CION*GP1)
192
      UIP2=2.66E35*DIEL*DIEL*TPOWR*SQRT(0.412)/(0.532*CION*GP2)
      UIP3=2.66E35*DIEL*DIEL*TPOWR*SQRT(0.246)/(0.253*CION*GP3)
      WEIGHT INDIVIDUAL MOBILITIES BY HOLE DENSITY IN THAT BAND
С
      UIP=(UIP1+UIP2*(0.412/0.568)**1.5+UIP3*EXP(-0.044/CAYT)*(0.246/0.5
196
     268)**1.5)/(1.+(0.412/0.568)**1.5+EXP(-0.044/CAYT)*(0.246/0.568)**1
     3.5)
      CALCULATE GAMMA FOR EFFECT OF H-H SCATTERING ON ION. IMP. MOBILITY
С
      IF (CPSTAR.LE.O.) GAMMA=0.632
```

```
IF (CPSTAR.LE.O.) GO TO 200
      IF (SUMIA.LE.O.) GAMMA=0.432
      IF (SUMIA.GT.O.) GAMMA=(SUMIA/CPSTAR)*(1.-EXP(-CPSTAR/SUMIA))
198
      IF (GAMMA.LT.0.432) GAMMA=0.432
200
      UIP=GAMMA*UIP
      IF (UIP.LE.O.) RATIOP=1.E6
      IF (UIP.LE.O.) GO TO 210
208
      RATIOP=6.*ULP/UIP
210
      XP=SQRT(RATIOP)
С
      COMBINE LATTICE AND IONIZED IMPURITY SCATTERING BY THE MIXED-
С
             SCATTERING FORMULA OF DEBYE AND CONWELL, PHYS. REV. 93,
             698-706 (1954). SUBROUTINE SICI PERFORMS THIS FUNCTION
С
      CALL SICI (SI,CI,XP)
214
      UDP=ULP*(1.0+RATIOP*(CI*COS(XP)+SIN(XP)*(SI-1.5707963)))
      OUT11 = UDP
С
      ADD ON THE EFFECTS OF NEUTRAL IMPURITY SCATTERING
С
      NEUTRAL IMPURITY MOBILITY AS PER ERGINSOY, PHYS REV 79,1013 (1950)
С
      UNIS = 0.02*PI**3*Q**3*MASS/(5*DIEL*CNUT*H**3)
С
      VALENCE BAND OF SILICON HAS THREE SEPARATE COMPONENTS
С
             PROCEDURE TAKEN FROM LI, NBS SPECIAL PUBLICATION 400-47
С
             FOR THIS CALCULATION, MASS VALUES OF LI AT 300 K ARE USED
220
      UNIS1=1.60E12*0.568/(DIEL*CNUT)
      UNIS2=1.60E12*0.412/(DIEL*CNUT)
      UNIS3=1.60E12*0.246/(DIEL*CNUT)
С
      SCLAR'S CORRECTION TO UNIS, SEE PHYS REV 104, 1559, (1956)
221
      EI1=0.71*0.568/((DIEL/1.1121E-10)**2*CAYT)
      EI2=0.71*0.412/((DIEL/1.1121E-10)**2*CAYT)
      EI3=0.71*0.246/((DIEL/1.1121E-10)**2*CAYT)
222
      UNIS1=UNIS1*0.82*(2.*SQRT(1./EI1)/3.+SQRT(EI1)/3.)
      UNIS2=UNIS2*0.82*(2.*SQRT(1./EI2)/3.+SQRT(EI2)/3.)
      UNIS3=UNIS3*0.82*(2.*SQRT(1./EI3)/3.+SQRT(EI3)/3.)
С
      WEIGHT INDIVIDUAL MOBILITIES BY HOLE DENSITY IN THAT BAND
224
      UNIS=(UNIS1+UNIS2*(0.412/0.568)**1.5+UNIS3*EXP(-0.044/CAYT)*(0.246
     2/0.568)**1.5)/(1.+(0.412/0.568)**1.5+EXP(-0.044/CAYT)*(0.246/0.568)
     3) \times 1.5)
226
      UDP=1/(1/UDP+1/UNIS)
С
      THAT COMPLETES THE COMPUTATION OF THE HOLE MOBILITY
      IF (CN.LE.O..AND.CP.LE.O.) GO TO 230
      RH=((CP*UDP*UDP-CN*UDN*UDN)/(Q*(CP*UDP+CN*UDN)))/(CP*UDP+CN*UDN)
      SIGMA = Q * (CN * UDN + CP * UDP)
      RHO=1./SIGMA
      UD=(CN*UDN+CP*UDP)/(CN+CP)
С
      END OF THE MOBILITY AND RELATED COMPUTATIONS
С
С
      UPON RETURNING, ISTAT INDICATES THE STATUS OF THE COMPUTATIONS
             FIRST DIGIT UNITY,
THIRD DIGIT UNITY,
FIFTH DIGIT 1 OR 2,
С
                                         CNSTAR WAS EQUAL TO ZERO
С
                                          CPSTAR WAS EQUAL TO ZERO
С
                                          BORN APPROXIMATION NOT VALID
С
      9.999999E19 IS A LARGE NUMBER INTRODUCED TO AVOID ZERO DIVISORS
С
230
      RETURN
      END
```

```
SUBROUTINE SICI(SI,CI,X)
С
      THIS ROUTINE COMBINES LATTICE AND IONIZED MOBILITY SCATTERING
С
С
             ACCORDING TO THE MIXED-SCATTERING FORMULA OF DEBYE AND
С
             CONWELL, PHYS. REV. 93, 693-706 (1954)
С
С
      TEST ARGUMENT RANGE
      Z = ABS(X)
      IF (Z-4.) 10,10,50
      Z IS NOT GREATER THAN 4.
С
10
      Y=Z*Z
      SI=X*(((((((,97942154E-11*Y-.22232633E-8)*Y+.30561233E-6)*Y-.283414
     260E-4 + 16666582E-2 + Y- 55555547E-1 + Y+1.)
С
      TEST FOR LOGARITHMIC SINGULARITY
      IF (Z) 30,20,30
      CI=-1.E38
20
      RETURN
      CI=0.57721566+AL0G(Z)-Y*(((((-.13869851E-9*Y+.26945842E-7)*Y-.3095
30
     22207E-5)*Y+.23146303E-3)*Y-.10416642E-1)*Y+.24999999)
      RETURN
40
      Z IS GREATER THAN 4.
С
      SI=SIN(Z)
50
      Y=COS(Z)
      Z=4./Z
      U=((((((((((((40480690E-2*Z-.022791426)*Z+.055150700)*Z-.072616418)*Z
     2+.049877159)*Z-.33325186E-2)*Z-.023146168)*Z-.11349579E-4)*Z+.0625
     300111) * Z+, 25839886E-9
      V=((((((((((-.0051086993*Z+.028191786)*Z-.065372834)*Z+.079020335)*
     2Z-.044004155)*Z-.0079455563)*Z+.026012930)*Z-.37640003E-3)*Z-.0312
     324178) * Z-.66464406E-6) * Z+.25000000
      CI=Z*(SI*V-Y*U)
      SI=-Z*(SI*U+Y*V)+1.5707963
      TEST FOR NEGATIVE ARGUMENT
С
      IF (X) 60,40,40
      X IS LESS THAN -4.
С
60
      SI=-SI
      RETURN
      END
```

5. Illustrative Output Data Cards and Examples

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	1.00000E15	0.045	2.
DUMMY			
DUMMY			
BORON	1.00000E13	0.045	4.
DUMMY			
DOUBLE ON			
PHOSPHORUS	1.00000E18	0.045	2.
DUMMY			
DUMMY			
BORON	1.00000E13	0.045	4.
DUMMY			
DOUBLE OFF			
DOLOOP A2	5.00000E14	4.	
PHOSPHORUS	1.00000E15	0.045	2.
DUMMY			
DUMMY			
BORON		0.045	4.
DUMMY			
CONSTANTS			
STOP			

5.2 Illustration of a No-Option Output

ELECTRICAL PROPERTIES CF SILICCN

DOPANT STATES FOR THIS FUN

	A2 10N	£1+000*1	1.000413	1 •000 + 1 3	1-000+13	1.000+13	1.000+13	1.000+13	1.000413	1.000+13	1.000+13	1+000+13	1+000+13	1.000+13	1,000+13	1.000413	1.000413	1.000+13	1.000+13	1.000+13	1.000+13	1.000+13	1.000+13	1.000+13	1.000+13	1.000+13	1.000+13	1.000+13	1.000+13	1.000+13	1.000+13	1.000+13	1.000+13	1 • 000 + 13	1+000+13
	A1 ION																																		
	D2 ION																																		
	DI ION	1.001+13	1.001+13	1.001+13	1.001+13	1.000+13	1.002+13	1.005+13	1.013+13	1.034+13	1.100+13	1.266+13	1.633+13	2.349+13	3.664+13	6.007+13	1.009+14	1.701+14	2.828+14	4.498+14	6.561+14	7.571+14	8.403+14	9.034+14	9.454+14	9.708+14	9.851+14	9.927+14	9.965+14	9.965+14	9.994+14	9.997+14	9.998+14	9.999+14	9.999+14
	RHO		6.317+05	2.143+05	7.264+04	2.457+04	8.340+03	2.830+03	9.661+02	3.351+02	1.219+02	4.870+01	2.227+01	1.162+01	6.729+00	4.201+00	2.762+00	1.889+00	1.342+00	9.936-01	7.868-01	7.265-01	6.942-01	6.855-01	6.999-01	7.509-01	8.772-01	1.077+00	1.406+00	1.991+00	3.143+00	4.651+00	5.863+00	8.811+00	1.333+01
DEGENERACY 2.0000 4.0000	RH		-3.722+10	-1.255+10	-4.217+09	-1.412+09	-4.727+08	-1.578+08	-5.273+07	-1.779+07	-6.223+06	-2.347+06	-5.879+05	-4.620+05	-2.340+05	-1.248+05	-6.877+04	-3.895+04	-2.287+04	-1.418+04	-9.661+03	-8.355+03	-7.520+03	-6.987+03	-6.€74+03	-6.498+03	-6.402+03	-6.351+03	-6.327+03	-6.315+03	-6.308+03	-6.307+03	-6.306+03	-6.305+03	-5.604+03
(CALC.)	COND. MOB		5.892+04	5.855+04	5.80€+04	5.745+04	5.666+04	5.574+04	5.458+64	5.310+04	5.106+04	4°812+04	4 ° 435+04	3.977+04	3.477+04	2.571+04	2.450+04	2.062+04	1.704+04	1.426+04	1.228+04	1.150+04	1.083+04	1.015+04	9 • 536 + 03	8.652+03	7.298+03	5.894+03	4°454+03	3.172+03	2.007+03	1.356+03	1.076+03	7.156+02	4.102+02
ENERGY • 044 • 041	٩																												2.471-12	3.802-06	7.199+00	1.298+05	1.864+07	3.591+10	7.592+13
VERGY (INPUT) • 0450 • 0450	z		1.677+08	4.975+08	1.480+09	4.421+09	1.320+10	3.956+10	1.184+11	3.508+11	1.003+12	2.660+12	6.318+12	1.351+13	2.667+13	5.001+13	9°076+13	1.602+14	2.729+14	4.400+14	6.460+14	7.470+14	8.300+14	8.932+14	9.352+14	9.606+14	5°749+14	9.828+14	9.864+14	9.884+14	9.894+14	9.896+14	9.898+14	5 . 899 + 14	1.066+15
ITY Er 0+15 0+13	L U	1.112868	1.118368	1.118646	1.118947	1.119274	1.119629	1.120014	1.120424	1 • 120841	1.121204	1.121352	1.121266	1.120762	1.115665	1.118632	1.116957	1。114741	1.111751	1.107547	1.101318	1.096569	1.091650	1.084869	1.076284	1.065316	1.051058	1.032014	1.005587	•966915	• 905922	.842058	•798308	• 708477	•573314
DENS 1.000 1.000	1000/1	238.0952	50,0000	48.0000	46.0000	44.0000	42.0000	40.0000	38,0000	36.0000	34.0000	32.0000	30.0000	28.0000	26.0000	24.0000	22.0000	20.0000	18.0000	16.0000	14.0000	12.9870	12.0000	11.0000	10.0000	9*0000	8.0000	7.0000	6 • 0000	5.0000	4.0000	3,3333	3*0000	2.5000	2.0000
DOPANT FHCSPHORLS BORCN	TEMP	4.2000	20.0000	20 . 83 33	21 • 7351	22.7273	23.8055	25.0000	26.3158	27.7778	29.4118	31.2500	33° 33 33	35.7143	28 4 6 15	41.6667	45.4545	50.0000	55.5556	62 . 5000	71.428€	77.0000	83, 5333	1506*05	100.0000	111.1111	125.0000	142.8571	166.6667	200.0000	250+0000	300.0000	223•3323	400.0000	500 • 00 00

5.3 Illustration of the DOUBLE ON Option Output

ELECTRICAL PROPERTIES OF SILICCN

DCPANT STATES FCR THIS FUN

	A2 10N	+NEUTRAL	1.000+13 4.596+02	1 •000+1 5 +02 4 • 853+02	1。000+13 4。838+02	1。000+13 4.820+02	1 •000+13 4 • 796+02	1.000+13 4.765+02	1。000+13 4.725+02	1.000+13 4.675+02	1。000+13 4.613+02	1.000+13 4.536+02	1.000+13 4.443+02
	A1 10N	+ I 0N 1 ZED	1•833+03	1 • 866+04	1 • 551 +04	1 • 278+04	1。044+04	8.490403	6.874+03	5+63+03	4.482+03	3.616403	2.922+03
	D2 10N	408+ (LAT)	1 • 755+06	1.587+05	1.490+05	1.396+05	1.302+05	1.213+05	1.125+05	1.040+05	9.568+04	8.762+04	7.581+04
	N01 10	+ NEUTRAL	1 •005+13 3 • 399+02	1。273+14 3。262+02	1.807+14 3.274+02	2。576+14 3。285+02	3.687+14 3.296+02	5°297+14 3•304+02	7.631+14 3.311+02	1。102+15 3。314+02	1 • 557 + 15 3 • 312 + 02	2.320+15 3.305+02	3.378+15 3.292+02
	КНО	+IONIZED	1.534+29 2.761+04	1.627+02 2.158+04	1.115+02 1.784+04	7.657+01 1.463+04	5.268+01 1.193+04	3.627+01 9.676+03	2。498+01 7.826+03	1.721+01 6.318+03	1.185+01 5.057+03	8.167+00 4.113+03	5。624+00 3。324+03
DEGENERACY 2.0000 4.0000	ня	M08-(LAT)	-5.212+31 1.886+06	-5.306+04 1.759+05	-3。650+04 1。653+05	-2.516+04 1.550+05	-1。736+04 1。449+05	-1.199+04 1.350+05	-8.271+03 1.253+05	-5•703+03 1•159+05	-3.526+03 1.068+05	-2.700+03 9.790+04	-1.851+03 8.928+04
(CALC。) 36 0	COND. MOB	SIGMA	3° 352+02 6° 521-30	3。262+02 6。147-03	3.274+02 8.570-03	3。285+02 1。30 6- 02	3。296+02 1。898-02	3.304+02 2.757-02	3-311+02 4-003-02	3.314+02 5.811-02	3.312+02 8.436-02	3.305+02 1.224-01	3.292+02 1.778-01
ENERGY • 026 • 009	۵.	A3 ION											
NERGY (1NPUT) • 0450 • 0450	z	EG-EF	1 • 197-13 • 246486	1.176+14 .143045	1.710+14 .143386	2。481+14 。143844	3•595+14 •144425	5。208+14 。145134	7.546+14 .145578	1。094+15 。146976	1.590+15 .148151	2.312+15 •149547	3.372+15 •151186
51TY E 00+18 00+13	L L	KT/Q	1.131032 3.6193-04	1.141563 1.7235-03	1.141527 1.7953-03	1.141478 1.8733-03	1.141415 1.5585-03	1.141337 2.0517-03	1.141243 2.1543-03	1.141130 2.2677-03	1.140954 2.3937-03	1.140830 2.5345-03	1.140633 2.6925-03
1 • 00	1000/T	TEST	238°0952 4°801+05	50•0000 -9•836+09	48.0000 -1.012+11	46.0000 -5.534+10	44.0000 -2.991+05	42.0000 -4.245+09	40 .0 000 -5.964+09	38°0000 -1°441+10	36.0000 -6.610+09	34.0000 -1.698+12	32.0000 -1.437+12
OOPANT Phcsphcrls Boron	TEMP	EG	4.2000 1.155681	20.0000 1.155867	20.8333 1.155866	21.7351 1.155863	22•7273 1•155858	23.8055 1.155851	25.0000 1.155841	26.3158 1.155827	27.7778 1.155809	29.4116 1.155785	31.2500 1.155752

1.000+13 4.333+02	1 • 000+13 4 • 205+02	1.000+13 4.060+02	1 • 000 + 1 3 3 • 900 + 02	1 • 000 + 1 3 3 • 7 29 + 0 2	1.000+13 3.551+02	1.000+13 3.373+02	1.000+13 3.201+02	1 • 000 + 1 3 3 • 0 4 5 + 0 2	1.000+13 2.966+02	1.000+13 2.892+02	1.000+13 2.820+02	1.000+13	1.000+13 2.690+02	1+000+13
2.367+03	1,922+03	1.567+03	1.284+03	1.058+03	8.777+02	7.335+02	6.184+02	5 • 267 + 0 2	4.851+02	4 • 484+02	4.143+02	3•838402	3•556+02	
7.226+04	6.457+04	5.797+04	5.124+04	4.482+04	3.870+04	3+290+04	2.744+04	2.234+04	1 • 854+04	1.498+04	1.184+04	9.156+03	6+689+03	
4.932+15 3.270+02	7.230+15 3.240+02	1.063+16 3.200+02	1 •569+16 3 • 152+02	2.325+16 3.095+02	3.459+16 3.033+02	5.172+16 2.970+02	7.768+16 2.911+02	1.171+17 2.866+02	1.445+17 2.852+02	1.773+17 2.848+02	2.182+17 2.856+02	2.682+17 2.879+02	3.292+17 2.920+02	4.025+17
3.872+00 2.694+03	2.667+00 2.189+03	1.836+00 1.787+03	1.264+00 1.465+03	E.686-01 1.209+03	5.956-01 1.005+03	4.069-01 8.419+02	2.763-01 7.119+02	1.859-01 6.089+02	1.515-01 5.654+02	1.236-01 5.282+02	1.002-01 4.954+02	E.078-02 4.673+02	6.491-02 4.429+02	5 •2 19 -0 2
-1.266+03 8.094+04	-8.641+02 7.288+04	-5.876+02 6.511+04	-3.984+02 5.765+04	-2.688+02 5.051+04	-1.806+02 4.370+04	-1。208+02 3。723+04	-8.042+01 3.113+04	-5。328+01 2。541+04	-4.321+01 2.267+04	-3.519+01 2.010+04	-2.862+01 1.761+04	-2。326+01 1。524+04	-1.895+01 1.266+04	-1.551+01
3.270+02 2.583-01	3.240+02 3.750-01	3.200+02 5.446-01	3.152+02 7.511-01	3.095+02	3.035+02 1.675+00	2.45E+00	2。511+02 3.615+00	2.866+02 5.37e+00	2.852+02 6.600+00	2.846+02 8.092+00	2.856+02 9.580+00	2.875+02 1.238+01	2•520+02 1•541+01	2+571+02
4.930+15 .153140	7.223+15 .155492	1.062+16 .158368	1 • 567+16 • 161915	2.322+16 .166363	3.455+16 •172063	5.166+16 •179550	7.761+16 .189694	1 • 1 7 1 + 1 7 • 203995	1 • 444+17 • 213633	1.773+17 .225213	2.181+17 .239965	2。683+17 。258918	3.293+17 .283882	4.025+17
1 • 1 40 3 5 5 2 • 87 2 4 - 0 3	1.140102 3.0776-03	l.139737 3.3143-03	1.139278 3.5905-03	1 • 1 38 6 89 3 • 9 1 7 0- 0 3	1.137919 4.3086-03	1.136855 4.7874-03	1.135452 5.3858-03	1.1333E6 6.1552-03	1.131972 6.6353-03	1.130252 7.1811-03	1.126037 7.8339-03	1.125161 8.6173-03	1.121334 5.5748-03	1.116066
11+161 •1-	28.0000 3.335+12	26.0000 1.730+12	24.0000 5.745+10	22+0000 2+2+12	20.0000 1.290+12	18.0000 5.057+11	16.0000 1.652+12	14.0000 -2.674+11	12.9870 -4.078+13	12+0000	11.0000 2.107+12	10.0000 -3.049+11	5.0000 -8.719+11	8.0000
33, 33 33 1 • 155 7 0 9	35.7143 1.155651	38.4615 1.155574	41.66667 1.155469	45.4545 1.155326	50.0000 1.155125	55556 1.154840	62.5000 1.154422	71.4226 1.153786	77.0000	63,3333 1,152773	50-5051 10-152034	100.0000	111.1111	125.0000

2•625+02	1 • 000 + 1 3 2 • 55 2 + 0 2	1。000+13 2。454+02	1。000+13 2。295+02	1.000+13 2.011+02	1.000413	1.000+13 1.518+02	1.000+13	1.000+13 6.072+01
3。294+02	3.041+02	2.782+02	2.485+02	2 • 09 7 + 02	1.749+02	1.542+02	1.190+02	8 • 055+01
5.013+03	3.495+03	2•305+03	1.409+03	7.714+02	4.715+02	3.548+02	2.169+02	1.187+02
2.971+02	4.888+17	5.870+17	6.929417	7•576+17	8•604+17	8,883+17	9.245+17	9.534+17
	3.042+02	3.129+02	3.206402	3•193+02	3•046+02	2,899+02	2.552+02	2.031+02
4.201+02	4.196-02	3。397-02	2.809-02	2.451-02	2,382-02	2.424-02	2•645-02	3=224-02
	4.010+02	3。846+02	3.685+02	3.457+02	3,192+02	2.998+02	2•598+02	2•046+02
9 • 630+03	-1。277+03	1.063+01	-9 • 006 + 0 0	-7.825+00	-7.255+00	-7。027+00	-6.751+00	-6。547+00
	7。065+03	4.940+03	3 • 236 + 0 3	1.929+03	1.263+03	9。894+02	6.482+02	3。862+02
1•516+01	3•042+02	3.125+02	3.20€+02	3,193+02	3.046+02	2.895402	2.552+02	2.031+02
	2•383+01	2.544+01	3.560+01	4,081+01	4.195+01	4.12€401	3.780+01	3.102+01
		4 • 099-15	5.362-09	8.849-03	1 • 482 + 02	2.065+04	3.826+07	8.460+10
•317754	4。889+17	5。871+17	6.930+17	7.976417	8•603+17	8+832+17	9.246+17	9.534+17
	•365459	。435719	.545392	•730403	•934975	1+080213	1.388266	1.884956
1.0772-02	1.106624	1.057527	1.080042	1.050250	1.017244	•953800	•944352	•866288
	1.2310-02	1.4362-02	1.7235-02	2.1543-02	2.5852-02	2•8724-02	3•4469-02	4•3086-02
4•933+13	7.0000 -7.813+12	6.0000 	5.0000 -1.477+12	4.0000 -1.155+13	3•3333 2•422+12	51+05E•1	2+5000 -4+255+12	2+0000 8+332+11
1.147862	14208571	166.6667	200 .0 000	250+00C0	300 • 00 00	333,3323	400°9000	500°0000
	10145170	1.141058	1.134581	1-123330	1 • 110741	1 • 101821	1•083219	1°054783

5.4 Illustration of the DOLOOP XX Option Output

ELECTRICAL PROPERTIES OF SILICON

DOPANT STATES FOR THIS FUN

A2 ION

	A1 ION																																		
	D2 ION																																		
	DI ION	4.756~12	3.286+10	5.709+10	9.942+10	1.732+11	3.024+11	5.287+11	9.280+11	1.629+12	2.864+12	5.045+12	8.917+12	1.576+13	2.793+13	4.951+13	8.735+13	1.524+14	2.602+14	4.236+14	6.322+14	7.375+14	8.260+14	8°943+14	9.403+14	9.682+14	9.838+14	9.921+14	9.963+14	9.984+14	9°663+14	9.996+14	9.998+14	9.999+14	9*999+14
	вно	4.382+24	1.558+03	9.368+02	5.659+02	3.432+02	2.094+02	1.287+02	7.985+01	4.592+01	3.154+01	2.016+01	1.308+01	8.552+00	5.741+00	3*901+00	2.693+00	1.890+00	1.358+00	1.007+00	7.931-01	7.290-01	6.932-01	6.818-01	6.541-01	7.435-01	8.679-01	1.066+00	1.353+00	1.970+00	3.111+00	4.603+00	5.803+00	8.722+00	1.321+01
EGENERACY 2.0000 4.0000	ЯН	-1 • 258+30	-1.856+08	-1.091+08	-6.270+07	-3.596+07	-2.060+07	-1.178+07	-6.738+06	-3.839+06	-2.182+06	-1.237+06	-7.010+05	-3.955+05	-2.233+05	-1.262+05	-7.152+04	-4.091+04	-2.398+04	+0+274.04	-9.873+03	-8.465+03	-7.559+03	-6.580+03	-6.639+03	-6.448+03	-6.345+03	-6.290+03	-6.265+03	-6.252+03	-6.245403	-6.244+03	-6.243+03	-6.242+03	-5.559+03
CALC.) D	COND. MOB	2.563+05	1.217+05	1 • 164+05	1.108405	1.046+05	9.835+04	9.156+04	8.435+04	7.691+04	6.515+04	6.137+04	5.356+04	4.603+04	3.885+04	3.235+04	2.656+04	2.164+04	1.766+04	1.462+04	1.245+04	1.161+04	1 • 050+04	1.024+04	9.565+03	8.673+03	7.311+03	5.502+03	E0+554 ° 4	3.174+03	2.008+03	1.356+03	1.076+03	7.156+02	4.105+02
ENERGY (• 0450 • 0414	٩																												2.447-12	3.764-06	7.127+00	1.285+05	1.846+07	3.555+10	7.526+13
ERGY (INPUT) •0450 •0450	z	4.807-12	3.291+10	5.722+10	9.955+10	1.736+11	3.030+11	5.258+11	9.262+11	1.626+12	2.860+12	5.044+12	8.904+12	1.578+13	2.795+13	4.945+13	8.727+13	1.526+14	2.603+14	4.238+14	6.322+14	7.374+14	8.257+14	8.942+14	9.401+14	9.630+14	9.836+14	9.922+14	9。962+14	9.963+14	5.994+14	9.996+14	9 . 998+14	9.999414	1.075+15
TY EN	EF	1.132364	1.127463	1.127160	1.126827	1.126460	1.126053	1.125559	1.125050	1.124516	1.123863	1.123115	1.122251	1.121240	1.120040	1.118552	1.116803	1.114529	1.111523	1.107345	1.101184	1.056882	1.091613	1.084877	1.076325	1.065389	1.051154	1.032132	1.005729	. 567087	.906138	.842357	°798556	.705824	•573650
DENS1 0.0000	1000/T	236.0952	50.0000	46.0000	46.0000	44.0000	42.0000	40.0000	38.0000	36.0000	34.0000	32.0000	30.0000	26.0000	26.0000	24+0000	22.0000	20.0000	18.0000	16.0000	14.0000	12.9870	12.0000	11.0000	10.0000	0000*5	8.0000	7.0000	6.0000	5.0000	4.0000	3,5333	3°0000	2.5000	2.0000
DOPANT PHCSPHORLS BORCN	TEMP	4.2000	20.0000	20.8333	21.7351	22.7273	23.8055	25.0000	26.3158	27.7778	29.4118	31.2500	53.3353	35°7143	38.4615	41.6667	45. 4545	50.0000	55+5556	£2.5000	71.4266	77.0000	83•3333	50° 00 5 1	100.0000	111.1111	125.0000	142.8571	166.6667	200.0000	250.0000	300.0000	323, 3333	400.0000	500.0000

DOPANT STATES FCR THIS RUN

с. С.	1
CUNU. M 4.105+	4 CUNU. 3
6.7564	6.7561
7.017	2 • 0 1 7 +
1.293+	7 + 293+
7.586+	7.586+
1.854+	7.854+
8.215+	8.215+
8.556+	8 . 558+
+E15*8	+E15*8
6°275+	6°215+
9.657+	9.657+
1 - 004+	1 - 004+
1.041+	1001
1 • 106+	1 • 106+
1.125+	1.125+
1.1334	1.1334
1.1124	1 • 1 12+
1.066	1.066
1.0154	1.0154
9.850+	9 8 8 0 +
9°632+	+0 -0 -0 -0 -0 -0 -0 -0 -0 -0 -0 -0 -0 -0
9.157+	9.157+
8.707+	8 • 707+
8.0154	8.0154
6.860+	6.860+
5.615+	5.615+
12 4.335+	4.890-12 4.335+
06 3.094+	7.526-06 3.094+
+272+1 10	1.425+01 1.577+
05 1.343+	2.570+05 1.343+
07 1.067+	3.692+07 1.067+
10 7.121+(7.109+10 7.121+(
14 3.767+	1. 20741A 3 7474

.

DOPANT STATES FCR THIS RUN

	A2 10N	1.000+15	1.000415	1.000+15	1.000+15	1.000+15	1 • 0 0 0 + 1 5	1.000+15	1.000+15	1.000+15	1 • 000 + 1 5	1.000+15	1.000+15	1.000+15	1.000+15	1.000+15	1.000+15	1.000+15	1.000+15	1.000+15	1.000+15	1.000+15	1 • 000 + 15	1.000+15	1.000+15	1.000+15	1.000+15	1.000+15	1.000+15	1.000+15	1.000+15	1 • 0 0 0 + 1 5	1.000+15	1.000+15	6°666+14
	AI ION																																		
	D2 10N																																		
	OI ION	1.000+15	1.000+15	1.000+15	1.000+15	1.000+15	1.000+15	1.000+15	1.000+15	1.000+15	1.000+15	1.000+15	1.000+15	1.000+15	1.000+15	1.000+15	1.000+15	1.000+15	1.000+15	1.000+15	1.000+15	1.000+15	1.000+15	1.000+15	1.000+15	1.000+15	1.000+15	1.000+15	1 • 000 + 15	1.000+15	1.000+15	1.000+15	1.000+15	1.000+15	1.000+15
	вно	2.188+01	2.188+01	2.168+01	2.188+01	2.188+01	2.188+01	2.188+01	2.188+01	2.188+01	2.188+01	2.188+01	2.188+01	2.188+01	2.168+01	2.168+01	2.188+01	2.188+01	2.188+01	2.188+01	2.188+01	2.188+01	1.984+29	2.078+26	2.131+23	2.164+20	2.235+17	2.358+14	2.613+11	4.718+05	2.913407	3.158+05	3,310+04	1.137+03	4.017+01
1666 NERACY 2.0000 4.0000	ня	-8.763+03	-8.763+03	-8.763+03	-8.763+03	-8.763+03	-8.763+03	-8.763+03	-8.763+03	-8.763+03	-8.763+03	-8.763+03	-8.763+03	-8.763+03	-8.763+03	-8.763403	-8.763+03	-8.763+03	-8.763+03	-8.763+03	-8.763+03	-8.763+03	-2.671+32	- 3.293+29	-3.971+26	-4.677+23	-5.366+20	-5.593+17	-6.530+14	4.758+12	-3.286410	-2.665+08	-2.317+07	-5.608+05	-1.247+04
(CALC.) (CONO. MOB	3.767+02	3.767+02	3.767+02	3.767+02	3.767+02	3.767+02	3.767+02	3.767+02	3.767+02	3.767+02	3.767+02	3.767+02	3.767+02	3.767+02	3.767+02	3.767+02	3.767+02	3.767+02	3.767+02	3.767+02	3.767+02	1.346+03	1.585+03	1.863+03	2.162+03	2.401+03	2.542+03	2.495+03	1.026+03	1.265+03	8.720+02	6.540+02	4.602+02	2.731+02
ENERGY (• 0414	C.																							7.236-17	8.571-14	1.043-10	1.317-07	1.758-04	2.550-01	1.236+06	8.474+07	1.133+10	1.358+11	5+961+12	2.844+14
NERGY (INPUT) • 0450 • 0450	z																						2.337-14	1.896-11	1.572-08	1.335-05	1.163-02	1.041+01	9.558+03	2.922403	8.405+07	1.133+10	1.359+11	5.963+12	2.845+14
ITY E 0+15 0+15	ц Ц	.600527	•603064	.603247	•603426	•603624	.603845	•604053	•604371	•604666	.605046	•605459	.605937	•606458	•607161	.607956	•608922	•610115	•611618	.613553	•616105	•617719	•619563	• 621767	•624367	627527	•631314	•635667	•641362	•5093E6	5555173	•547573	•542848	•5322€8	•5164 65
06NS 1 • 0 00	1000/T	238.0952	50.0000	48.0000	46.0000	44.0000	42.0000	40.0000	36.0000	36.0000	34.0000	32.0000	30,0000	28.0000	26.0000	24.0000	22.0000	20.0000	16.0000	16.0000	14.0000	12.9670	12.0000	11.0000	10.0000	0000*5	8.0000	7.0000	6.0000	5.0000	4.0000	3,3333	3+0000	2.5000	2.0000
DOPANT PHCSPHORLS BORCN	TEMP	4.2000	20.0000	20°8333	21.7391	22.7273	23.8055	25.0000	26.315E	27.7778	29.4118	31.2500	53,53,53 53,53 53,53 55,55 55,55 55,55 55,55 55,55 55,55 55,55 55,55 55,55 55,5555 55,55555 55,55555 55,55555 55,55555 55,555555	35.7143	38°4615	41.6667	45°4545	50.0000	55° 555 6	62.5000	71.4286	77.0000	63,3323	1506 05	100.0000	111.1111	125.0000	142.8571	166.6667	200.0000	250.0000	300°0000	50 50 50 50 50 50 50 50 50 50 50 50 50 5	400.0000	500.0000

DOPANT STATES FOR THIS RUN

DOPANT Phcsphorls Boron	DENSI 1 •000 1 •500	TY El +15 +15	NERGY (1NPUT) •0450 •0450	ENERGY =	cALC.)	DEGENERACY 2.0000 4.0000					
TEMP	1000/1	L L	z	٩	COND. MOB	ни Н	кно	NDI 10	D2 ION	A1 ION	A2 10N
4 • 2000	238.0552	.042157			2.731+02	-1.247+04	4°017+01	1 • 000 + 15			6 *998+14
20.0000	50.0000	•044568		8.949+05	3.895+03	6.974+12	1.791+09	1.000+15			9*998+1
20 8333	48.0000	•045137		2.488+06	4.050+03	2.509+12	6.194+08	1.000+15			9.998+14
21.7351	46.0000	•045300		6.930+06	4.216+03	9.006+11	2.136+08	1.000+15			1+000+15
22 + 7273	44.0000	•045477		1.937+07	4.352+03	3.223+11	7.337+07	1.000+15			1.000+15
23 80 55	42.0000	•045671		5.437+07	4.582+03	1.148+11	2.505+07	1.000+15			9*998+14
25.0000	40.0000	•045864		1.529+08	4.783+03	4 • C82+10	8.535+06	1.000+15			1 - 000+1
26.3158	38.0000	•046120		4°324+08	4 • 596+03	1.444+10	2,888+06	1.000+15			6 *999 + 14
27°778	36.0000	•046381		1。226+09	5.225+03	50+050°S	5°741+05	1.000+15			1.000+15
29.4118	34.0000	•046674		3.457+09	5.466+03	1.785+09	3.265+05	1.000+15			1.000+15
31.2500	32.0000	.047064		1.004+10	5.72C+03	6 • 220 + 08	1.087+05	1.000+15			6*999+14
53656565	30.0000	047377		2.894+10	5.584+03	2.156+08	3.604+04	1.000+15			1.000+15
35°7143	28.0000	•047805		8.413+10	6.255+03	7.419+07	1.186+04	1.000+15			1-000+1
38°4615	26.0000	•048259		2.465+11	6.530+03	2。532+07	3.877+03	1.000+15			1+000+15
41.6667	24.0000	•046679		7.293+11	6.758+03	8.558+06	1.255+03	1-000+15			1.001+15
45°4545	22 • 0 0 0 0	•049575		2.176+12	E0+5+0°2	2.869+06	4.070+02	1.000+15			1.002+15
50.0000	20.0000	0 50 4 4 8		6.525+12	7.255403	9.565+05	1.318+02	1.000+15			1.007+15
55°5556	18.0000	•051641		1.941+13	7°397+03	3.216+05	4.347+01	1.000+15			1.019+15
62.5000	16.0000	•053519		5.496+13	7.410+03	1.136+05	1.533+01	1.000+15			1.055415
71.4266	14.0000	•056942		1.360+14	7.237+03	4.550+04	6.342+00	1.000+15			1.136+15
77.0000	12.5870	•059737		1.977+14	6.808403	3.158+04	4.638+00	1.000+15			1.198+15
63•3346	12.0000	•063481		2。659+14	6.250+03	2.347+04	3.755+00	1.000+15			1.266+15
50° 30 5 1	11.0000	•068623		3。346+14	5.615+03	1 • 865+04	3.322+00	1.000+15			1.335+15
100.0000	10.0000	•075515		3.935+14	4.518+03	1.586+04	3.225+00	1.000+15			1.394+15
111.1111	5 • 0000	•084676		4.373+14	4.174+03	1.427+04	3.415+00	1.000+15			1.437+15
125.0000	8.0000	•056850		4.659+14	3.401+03	1 • 3 4 0 + 0 4	00+6E6°E	1.000+15			1.466+15
142.8571	7.0000	•113230		4.826+14	2.628403	1.293+04	4.921+00	1.000+15			1.483+15
166.6667	6 • 0000	•135882	4.957-12	4.917+14	1.896+03	1 • 269+04	6.696+00	1.000+15			1.492+15
200.0000	5.0000	•168641	7.572-06	4°963+14	1.247+03	1.258+04	1.008+01	1.000+15			1-496+15
250.0000	4 • 0000	•219370	1.429+01	4.984+14	7.223402	1.252+04	1.734+01	1.000+15			1.498+15
300.0000	3,3333	•271540	2.573+05	4°992+14	4.536+02	1 • 250+04	2.756401	1.000+15			1 • 499 + 15
333,3333	3.0000	• 307022	3.695+07	4°994+14	3.445+02	1.250+04	3.623+01	1.000+15			1 • 499 + 15
400.0000	2.5000	•375610	7.112+10	4.998+14	2.135+02	1 • 246+04	5.850+01	1.000+15			1.500+15
500.0000	2.0000	•482244	1.287+14	6.286+14	1.702+02	-5.517+03	4.843+01	1.000+15			1.500+15

5.5 Illustration of the CONSTANTS Option Output

ELECTRICAL PROPERTIES OF SILICON

T O O O I	NT 10	E C	0 TEL	AD B. (AT)	MORA (LAT)	「「日本日」	MC.			
	2	2					U E	Ē	•	2
095	2 3.6193-04	1.1557	11.4331	2.134+06	1.755+06	8.607+00	1.062+00	5.886-01	4.550+16	1.877+16
000	0 1.7235-03	1.1559	11.4472	1.990+05	1.587+05	8 • 94 4 + 0 1	1+062+00	5.867-01	4.727+17	1.941+17
000	0 1.7953-03	1.1559	11.4480	1.870+05	1.490+05	9.505+01	1.062+00	5.868-01	5.026+17	2.064+17
•000	0 1.8733-03	1.1559	11.4468	1.753+05	1.396+05	1.014+02	1.062+00	5.870-01	5.357+17	2.201+17
• 0 0 0	0 1.5585-03	1.1559	11.4497	1.639+05	1.303+05	1.083+02	1.062+00	5.871-01	5.728+17	2.354+17
.000	0 2.0517-03	1.1559	11.4506	1.527+05	1.213+05	1.162+02	1.062+00	5.874-01	6.143+17	2.525+17
•000	0 2.1543-03	1.1558	11.4517	1.418+05	1.125+05	1.250+02	1.062+00	5.876-01	6.610+17	2.719+17
• 0 0 0	0 2.2677-03	1.1558	11.4529	1.311+05	1.040+05	1.350+02	1.063+00	5.880-01	7.141+17	2.939+17
• 0 0 0	0 2.3937-03	1.1558	11.4542	1.208405	9.568+04	1.464+02	1.063+00	5.884-01	7.746+17	3.191+17
• 0 0 0	0 2.5345-03	1.1558	11.4557	1.107+05	8.762+04	1.595+02	1.063+00	5.889-01	8.443+17	3.481+17
.000	0 2.6929-03	1.1558	11.4573	1.010+05	7.981+04	1.747+02	1.063+00	5.896-01	5.250+17	3.819+17
• 0 0 0	0 2.8724-03	1 • 1 557	11.4592	9.156+04	7.226+04	1.925+02	1.064+00	5.904-01	1.020+18	4.216+17
000 * 0	0 3.0776-03	1.1557	11.4613	8.244404	6.457+04	2.134+02	1.064+00	5.915-01	1.132+18	4.688+17
	0 2.3143-03	1 • 1 556	11.4637	7.366+04	5.757+04	2.385+02	1.065+00	5.928-01	1.266+18	5.258+17
	0 3.5905-03	1.1555	11.4666	6.522+04	5.124+04	2.650+02	1.066+00	5.946-01	1.429+18	5.955+17
• 0 0 0	10 2.5170-C3	1.1553	11.4700	5.714+04	4.482+04	3.065+02	1 •067 +00	5.969-01	1.630+18	6.825+17
000*	0 4.3086-03	1.1551	11.4741	4043404	3.870+04	3.536+02	1.068+00	6.000-01	1.864418	7.936+17
000*8	0. 4 • 7874-03	1.1548	11.4750	4 • 2 1 2 + 0 4	3.290+04	4.141+02	1.070+00	6.042-01	2.213+18	9.392+17
\$ • 0 0 0	0 5.3858-03	1.1544	11.4853	3.521+04	2.745+04	4.941+02	1.072+00	6.100-01	2.649+18	1.137+1E
• • • •	0 6.1552-C3	1.1538	11.4933	2.875+04	2.224+04	6.037+02	1.076+00	6.181-01	3.253+18	1.417+18
2.987	0 6.6353-03	1 ° 1 5 3 3	11.4983	2.564+04	1.854+04	6.757+02	1.078+00	6.236-01	3.653+18	1.607+18
000.	0 7.1811-03	1.1528	11.5039	2.274+04	1.456+04	7.607+02	1.081400	6.300-01	4.128+18	1.837+18
000*1	0 7.8339-03	1.1520	11.5107	1.992+04	1.164+04	8.666402	1.084+00	6.379-01	4.727+18	2.132+1E
00000	0 8.6173-03	1.1511	11.5189	1.724+04	9.156+03	1.000403	1.089+00	6.476-01	5.466+18	2.517+18
000.5	0 5.5748-03	1.1497	11.5289	1.432404	6.889+03	1.171+03	1.094+00	6.558-01	6.474+18	3.031+18
9.000	00 1.0772-C2	1.1479	11.5414	1.085404	5.013+03	1.398+03	1.101+00	6.750-01	7.759+18	3.742+18
7.000	0 1.2310-02	1.1452	11.5575	2.952+03	3.455+03	1.707+03	1.110+00	6.540-01	9.647+18	4.767+18
6.000	0 1.4362-02	1.1411	11.5790	5.589+03	2.305+03	2.152+03	1.122+00	7.178-01	1.235+19	6.318+18
5.000	0 1.7235-02	1.1346	11.6091	3.661+03	1.405+03	2.828403	1.139+00	7.469-01	1.659+19	8.817+18
0000*	00 2.1543-C2	1.1233	11.6545	2.182+03	7.714+02	3.953+03	1.161+00	7.812-01	2.389+19	1.318+15
3,333	33 2.5852-02	1.1107	11.7000	1.429+03	4.715+02	5.196+03	1.182+00	8.071-01	3.225+19	1.820+19
000°E	0 2.8724-02	1.1018	11.7305	1.119+03	3.548+02	6.086+03	1.195+00	8.220-01	3.841+19	2.150+15
2.500	0 3.4469-02	1.0832	11.7916	7.332+02	2.169+02	8.000+03	1.221+00	8.507-01	5.214+19	3.031+15
2.000	0 4.3086-02	1.0548	11.8840	4.365+02	1.187+02	1.118+04	1.256+00	8.538-01	7.558+19	4.562+19

6. CONCLUSIONS

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.

ACKNOWLEDGMENTS

The authors would like to thank Thomas F. Leedy, William J. Keery, and Sheng S. Li (University of Florida) for many helpful discussions and suggestions during the development of this program. They would also like to thank David K. Kahaner for a critical review of the manuscript and for pointing out the availability of the subroutine ZEROIN and Jane Walters for preparing the manuscript for publication.

REFERENCES

- Larrabee, R. D., Interpretation of Hall Measurements, Semiconductor Characterization Techniques, Proceedings Volume 78-3, P. A. Barnes and G. A. Rozgonyi, Eds, pp. 71-76 (The Electrochemical Society, Princeton, 1978).
- Bullis, W. M., and Strieter, F. J., Electrical Properties of n-Type Silicon Doped with Gold, J. Appl. Phys. 39, 314-318 (1968).
- Thurber, W. R., Lewis, D. C., and Bullis, W. M., Resistivity and Carrier Lifetime in Gold-Doped Silicon, AFCRL Report AFCRL-TR-73-0107 (January 31, 1973).
- 4. Larrabee, R. D., "X" Levels in Indium-Doped Silicon, Proc. IRIS Specialty Group Meeting, Annapolis, Maryland, June 13-15, 1978.
- 5. Blakemore, J. S., Semiconductor Statistics, pp. 354-365 (Pergamon Press, New York, 1962).
- 6. McCracken, D. D., A Guide to Fortran IV Programming, pp. 87-89 (John Wiley and Sons, New York, third corrected printing, August, 1968).

- Barber, H. D., Effective Mass and Intrinsic Concentration in Silicon, Solid-State Electronics 10, 1039-1051 (1967).
- Macfarlane, G. G., McLean, T. P., Quarrington, J. E., and Roberts, V., Fine Structure in the Absorption-Edge Spectrum of Si, *Phys. Rev.* <u>111</u>, 1245-1254 (1958).
- 9. Penin, N. A., Zurkin, B. G., and Volkov, B. A., Influence of the Concentration of Donors and Acceptors on the Electrical Conductivity of Heavily Doped n-Type Silicon, Sov. Phys. Solid State 7, 2580-2584 (1966).
- Sclar, N., Resistivity and Deep Impurity Levels in Silicon at 300 K, IEEE Trans. Electron Devices ED-24, 709-712 (1977).
- 11. Shampine, L. F., and Watts, H. A., ZEROIN A Root-Solving Code, Sandia Report SC-TM-70-631, September 1970.
- Dekker, T. J., Finding a Zero by Means of Successive Linear Interpolation, Constructive Aspects of the Fundamental Theorem of Algebra, B. Dejon and P. Henrici, Eds., pp. 37-51 (Wiley-Interscience, London, 1969).
- 13. Shampine, L. F., and Allen, R. C., Jr., Numerical Computing: An Introduction, pp. 87-108, 242-246 (Saunders, Philadelphia, 1973).
- 14. Norton, P., Braggins, T., and Levinstein, H., Impurity and Lattice Scattering Parameters as Determined from Hall Mobility Analysis in n-type Silicon, *Phys. Rev. B* 8, 5632-5653 (1973).
- 15. Thurber, W. R., Mattis, R. L., Liu, Y. M., and Filliben, J. J., Resistivity-Dopant Density Relationship for Phosphorus-Doped Silicon, J. Electrochem. Soc. 127, 1807-1812 (1980).
- Braggins, T. T., Analysis of Carrier Concentration and Mobility in Boron-Doped Silicon, Ph.D. Thesis, University Microfilms International, Ann Arbor, Michigan (1975).
- Ludwig, G. W., and Watters, R. L., Drift and Conductivity Mobility in Silicon, *Phys. Rev.* 101, 1699-1701 (1956).
- Brooks, H., Theory of the Electrical Properties of Germanium and Silicon, Advances in Electronics and Electron Physics, L. Marton, Ed., Vol. 7, pp. 85-183 (Academic Press, New York, 1955).
- Herring, C., and Vogt, E., Transport and Deformation Potential Theory for Many-Valley Semiconductors with Anisotropic Scattering, *Phys. Rev.* 101, 944-961 (1956).
- 20. Li, S. S., and Thurber, W. R., The Dopant Density and Temperature Dependence of Electron Mobility and Resistivity in n-Type Silicon, Solid-State Electronics 20, 609-616 (1977).

- 21. Li, S. S., Semiconductor Measurement Technology: The Theoretical and Experimental Study of the Temperature and Dopant Density Dependence of Hole Mobility, Effective Mass, and Resistivity in Boron-Doped Silicon, NBS Special Publication 400-47 (November 1979).
- Debye, P. P., and Conwell, E. M., Electrical Properties of N-Type Germanium, *Phys. Rev.* 93, 693-706 (1954).
- Dunlap, W. C., Jr., and Watters, R. L., Direct Measurement of the Dielectric Constants of Silicon and Germanium, *Phys. Rev.* <u>92</u>, 1396-1397 (1953).
- 24. Cardona, M., Paul, W., and Brooks, H., Dielectric Constant of Germanium and Silicon as a Function of Volume, J. Phys. Chem. Solids <u>8</u>, 204-206 (1959).
- Erginsoy, C., Neutral Impurity Scattering in Semiconductors, *Phys. Rev.* 79, 1013-1017 (1950).
- Sclar, N., Neutral Impurity Scattering in Semiconductors, *Phys. Rev.* 104, 1559-1568 (1956).
- Neuberger, M., and Welles, S. J., Silicon, Electronic Properties Information Center, Hughes Aircraft Company, Culver City, California, October 1969, AD 698342.

FEDERAL	NFORMATION PRO	CESSING ST	NDARD SOFTW	ARE SUMMARY				
D1. Summary date 02. Summary Yr. Mo. Day R. D. Lar 05. Software 05. Software Q4. Software date A FORTRA Yr. Mo. Day	prepared by (Name and Phon rabee , W. R. Thu title N Program for Calc rs of Extrinsic Si	e) * rber*, and W. ulating the I licon	M. Bullis [#] Electrical	03. Summary action New Replacement Deletion XX				
06. Short title				07. Internal Software ID				
18. Software type 09. P	ocessing mode 10.		Application are					
Automated Data System I Gomputer Program Subroutine/Module	teractive Compo atch Suppo atch X Scient ombination Biblion	General uter Systems ort/Utility ific/Engineering graphic/Textual	Management/ Business Process Control Other	Specific Scientific Functional Evaluation				
"I. Submitting organization and a National Bureau of Electron Devices D Washington, DC 20	^{Idress} Standards ivision 234		12. Technical contact(R. D. Larr W. R. Thur W. M. Bull	s) and phone abee (301) 921-3625 ber (301) 921-3625 is (301) 921-3786				
nature and density of properties hinges on position of the Ferm presented that perfo- electrical parameters this program have pro- degree of ionization predicting the behav conceptually) changed different scattering	the active impur the solution of t level for each s ms this determina of silicon as a oven useful in int of the separate d or of specimens w d, and understandi mechanisms on car	ities present he charge bal pecific case tion and ther function of t erpreting Hal opant states hen the dopar ng the variat rier mobility	Calculation of interest. calculates so cemperature. R l effect data, as a function t picture is i ions in the re as the temper	a of these electrical to determine the A FORTRAN program is ome of the often-used Results obtained from determining the of temperature, ntentionally (or elative roles of the rature is changed.				
Carrier density; com mobility; resistivit	puter program; ele y; silicon.	ectrical prop	erties of silio	con; Hall effect;				
5. Computer manuf'r and model	16. Computer operating sy	ystem 17. Prog	raming language(s)	18. Number of source program state-				
UNIVAC 1108	UNIVAC 1100	FORT	RAN IV	700				
9. Computer memory requirement	s 20. Tape drives	21. Disk	/Drum units	22. Terminals				
	None	None		Printer				
3. Other operational requirements		I						
4. Software availability		25. Doc	umentation availability					
Available Limited In-house only Available Inadequate In-house only Image: See item 12 for contacts. Image: See item 12 for contacts. Image: See item 12 for contacts. Image: See item 12 for contacts. Image: See item 12 for contacts. Image: See item 12 for contacts. Image: See item 12 for contacts. Image: See item 12 for contacts. Image: See item 12 for contacts. Image: See item 12 for contacts. Image: See item 12 for contacts. Image: See item 12 for contacts. Image: See item 12 for contacts. Image: See item 12 for contacts. Image: See item 12 for contacts. Image: See item 12 for contacts. Image: See item 12 for contacts. Image: See item 12 for contacts. Image: See item 12 for contacts. Image: See item 12 for contacts. Image: See item 12 for contacts. Image: See item 12 for contacts. Image: See item 12 for contacts. Image: See item 12 for contacts. Image: See item 12 for contacts. Image: See item 12 for contacts. Image: See item 12 for contacts. Image: See item 12 for contacts. Image: See item 12 for contacts. Image: See item 12 for contacts. Image: See item 12 for contacts. Image: See item 12 for contacts. Image: See item 12 for contacts. Image: See item 12 for contacts.								
5. FOR SUBMITTING ORGANIZAT	ION USE			Standard Form 185 1974 July U.S. Dept. of Commerce—NBS				

NB5-114A (REV. 2-80)		12 Desfermine Orace Data All 1 2	Dublication Data
U.S. DEPT. OF COMM.	REPORT NO.	2. Penonning Organ. Report No. 3	- Fublication Date
SHEET (See instructions)	NBS SP 400-63		October 1980
4. TITLE AND SUBTITLE			······································
<i>Semiconductor Meas</i> Electrical Paramet	urement Technology: ers of Extrinsic Sili	A FORTRAN Program for Ca con	lculating the
5. AUTHOR(S)			
R. D. Larrabee, W.	R. Thurber, and W. M	. Bullis	
6. PERFORMING ORGANIZA	TION (If joint or other than NBS	, see instructions) 7.	Contract/Grant No.
NATIONAL BUREAU OF			
DEPARTMENT OF COMM	ERCE	8.	Type of Report & Period Covered
WASHINGTON, D.C. 2023	4		Final
			Final
9. SPONSORING ORGANIZA	ITON NAME AND COMPLETE A	DUKESS (Street, City, State, ZIP)	
Same as No. 6			
	-		
X Document describes a	a computer program; SF-185, FIP	S Software Summary, is attached.	
 ABSTRACT (A 200-word of bibliography or literature 	or less factual summary of most survey, mention it here)	significant information. If document	includes a significant
Many electrical prop	perties of silicon are	strongly dependent upon	the specific nature
and density of the a	ctive impurities pres	ent. Calculation of the charge balance equation :	se electrical to determine the
position of the Ferm presented that perfor electrical parameter this program have pr degree of ionization predicting the behave conceptually) change different scattering	i level for each spec orms this determination of silicon as a fun- oven useful in interp of the separate dopa vior of specimens when ed, and understanding g mechanisms on carrie	ific case of interest. A n and then calculates son ction of temperature. Re reting Hall effect data, nt states as a function of the dopant picture is in the variations in the rear r mobility as the tempera	A FORTRAN program is me of the often-used esults obtained from determining the of temperature, ntentionally (or lative roles of the ature is changed.
12. KEY WORDS (Six to twelv	e entries; alphabetical order; ca	pitalize only proper names; and sep	arate key words by semicolons)
Carrier density; com mobility; resistivit	mputer program; electr y; silicon.	ical properties of silico	on; Hall effect;
13. AVAILABILITY			14. NO. OF
X Unlimited			PRINTED PAGES
For Official Distribut	ion. Do Not Release to NTIS		54
X Order From Superinter	ident of Documents, U.S. Govern	ment Printing Office, Washington, D	C 15 Price
20402.			
Order From National	Fechnical Information Service (N	TIS), Springfield, VA. 22161	\$3.75
		,	USCOMM-DC 6043-P80





Subscribe now— The new National Bureau of Standards Journal

The expanded Journal of Research of the National Bureau of Standards reports NBS research and development in those disciplines of the physical and engineering sciences in which the Bureau is active. These include physics, chemistry, engineering, mathematics, and computer sciences. Papers cover a broad range of subjects, with major emphasis on measurement methodology, and the basic technology underlying standardization. Also included from time to time are survey articles on topics closely related to the Bureau's technical and scientific programs. As a special service to subscribers each issue contains complete citations to all recent NBS publications in NBS and non-NBS media. Issued six times a year. Annual subscriptions: domestic \$13.; foreign \$16.25. Single copy, \$3. domestic; \$3.75 foreign.

 Note: The Journal was formerly published in two sections: Section A "Physics and Chemistry" and Section B "Mathematical Sciences."

NBS Board of Editors Churchill Eisenhart, Executive Editor (Mathematics) John W. Cooper (Physics) Donald D. Wagman (Chemistry) Andrew J. Fowell (Engineering) Joseph O. Harrison (Computer Science) Howard J. M. Hanley (Boulder Labs.)

Subscription Order Form Enter my subscription to NBS Journal of Research at \$13. Add \$3.25 for foreign mailing. No additional postage is required for mailing within the United States or its possessions. (SJRA—File Code 2N) Send Subscription to:	Credit Card Orders Only Total charges \$
Name-First, Last Company Name or Additional Address Line	Remittance Enclosed. Domestic: Check or money order. Foreign: International money order, draft on an American or Canadian Bank, or by UNESCO coupons, Made payable to the Superintendent of Documents.
Street Address	Charge to my Deposit Account No.
City State (or) COUNTRY PLEASE PRINT	Zip Code MAIL ORDER FORM TO: Superintendent of Documents Government Printing Office Washington, D.C. 20402



NBS TECHNICAL PUBLICATIONS

PERIODICALS

JOURNAL OF RESEARCH—The Journal of Research of the National Bureau of Standards reports NBS research and development in those disciplines of the physical and engineering sciences in which the Bureau is active. These include physics, chemistry, engineering, mathematics, and computer sciences. Papers cover a broad range of subjects, with major emphasis on measurement methodology and the basic technology underlying standardization. Also included from time to time are survey articles on topics closely related to the Bureau's technical and scientific programs. As a special service to subscribers each issue contains complete citations to all recent Bureau publications in both NBS and non-NBS media. Issued six times a year. Annual subscription: domestic \$13; foreign \$16.25. Single copy, \$3 domestic; \$3.75 foreign.

NOTE: The Journal was formerly published in two sections: Section A "Physics and Chemistry" and Section B "Mathematical Sciences."

DIMENSIONS/NBS—This monthly magazine is published to inform scientists, engineers, business and industry leaders, teachers, students, and consumers of the latest advances in science and technology, with primary emphasis on work at NBS. The magazine highlights and reviews such issues as energy research, fire protection, building technology, metric conversion, pollution abatement, health and safety, and consumer product performance. In addition, it reports the results of Bureau programs in measurement standards and techniques, properties of matter and materials, engineering standards and services, instrumentation, and automatic data processing. Annual subscription: domestic \$11; foreign \$13.75.

NONPERIODICALS

Monographs—Major contributions to the technical literature on various subjects related to the Bureau's scientific and technical activities.

Handbooks—Recommended codes of engineering and industrial practice (including safety codes) developed in cooperation with interested industries, professional organizations, and regulatory bodies.

Special Publications—Include proceedings of conferences sponsored by NBS, NBS annual reports, and other special publications appropriate to this grouping such as wall charts, pocket cards, and bibliographies.

Applied Mathematics Series—Mathematical tables, manuals, and studies of special interest to physicists, engineers, chemists, biologists, mathematicians, computer programmers, and others engaged in scientific and technical work.

National Standard Reference Data Series—Provides quantitative data on the physical and chemical properties of materials, compiled from the world's literature and critically evaluated. Developed under a worldwide program coordinated by NBS under the authority of the National Standard Data Act (Public Law 90-396). NOTE: The principal publication outlet for the foregoing data is the Journal of Physical and Chemical Reference Data (JPCRD) published quarterly for NBS by the American Chemical Society (ACS) and the American Institute of Physics (A1P). Subscriptions, reprints, and supplements available from ACS, 1155 Sixteenth St., NW, Washington, DC 20056.

Building Science Series—Disseminates technical information developed at the Bureau on building materials, components, systems, and whole structures. The series presents research results, test methods, and performance criteria related to the structural and environmental functions and the durability and safety characteristics of building elements and systems.

Technical Notes—Studies or reports which are complete in themselves but restrictive in their treatment of a subject. Analogous to monographs but not so comprehensive in scope or definitive in treatment of the subject area. Often serve as a vehicle for final reports of work performed at NBS under the sponsorship of other government agencies.

Voluntary Product Standards—Developed under procedures published by the Department of Commerce in Part 10, Title 15, of the Code of Federa! Regulations. The standards establish nationally recognized requirements for products, and provide all concerned interests with a basis for common understanding of the characteristics of the products. NBS administers this program as a supplement to the activities of the private sector standardizing organizations.

Consumer Information Series—Practical information, based on NBS research and experience, covering areas of interest to the consumer. Easily understandable language and illustrations provide useful background knowledge for shopping in today's technological marketplace.

Order the above NBS publications from: Superintendent of Documents, Government Printing Office, Washington, DC 20402.

Order the following NBS publications—FIPS and NBSIR's—from the National Technical Information Services, Springfield, VA 22161.

Federal Information Processing Standards Publications (FIPS PUB)—Publications in this series collectively constitute the Federal Information Processing Standards Register. The Register serves as the official source of information in the Federal Government regarding standards issued by NBS pursuant to the Federal Property and Administrative Services Act of 1949 as amended, Public Law 89-306 (79 Stat. 1127), and as implemented by Executive Order 11717 (38 FR 12315, dated May 11, 1973) and Part 6 of Title 15 CFR (Code of Federal Regulations).

NBS Interagency Reports (NBSIR)—A special series of interim or final reports on work performed by NBS for outside sponsors (both government and non-government). In general, initial distribution is handled by the sponsor; public distribution is by the National Technical Information Services, Springfield, VA 22161, in paper copy or microfiche form.

BIBLIOGRAPHIC SUBSCRIPTION SERVICES

The following current-awareness and literature-survey bibliographies are issued periodically by the Bureau:

Cryogenic Data Center Current Awareness Service. A literature survey issued biweekly. Annual subscription: domestic \$35; foreign \$45.

Liquefied Natural Gas. A literature survey issued quarterly. Annual subscription: \$30.

Superconducting Devices and Materials. A literature survey issued quarterly. Annual subscription: \$45. Please send subscription orders and remittances for the preceding bibliographic services to the National Bureau of Standards, Cryogenic Data Center (736) Boulder, CO 80303.

U.S. DEPARTMENT OF COMMERCE National Bureau of Standards Washington, D.C. 20234

OFFICIAL BUSINESS

Penalty for Private Use, \$300

POSTAGE AND FEES PAID U.S. DEPARTMENT OF COMMERCE COM-215



SPECIAL FOURTH-CLASS RATE BOOK

·





