SPARCOL:
A Front End for the
MAIN2 Program

Richard L. Mattis

U.S. DEPARTMENT OF COMMERCE
National Institute of Standards
and Technology
Center for Electronics and Electrical
Engineering
Semiconductor Electronics Division
Gaithersburg, MD 20899

October 1990

NIST

DATE DUE

SPARCOL:
A Front End for the
MAIN2 Program

Richard L. Mattis

**U.S. DEPARTMENT OF COMMERCE
National Institute of Standards
and Technology
Center for Electronics and Electrical
Engineering
Semiconductor Electronics Division
Gaithersburg, MD 20899**

Table of Contents

SPARCOL: A Front End for the MAIN2 Program

by

Richard L. Mattis
Semiconductor Electronics Division
National Institute of Standards and Technology
Gaithersburg, Maryland 20899

1. INTRODUCTION

SPARCOL is an interactive program which serves as a front-end to the MAIN2 and MAIN2R computer programs. SPARCOL (pronounced "sparkle") stands for SPectroscopic ellipsometry And Reflectance for Characterization Of Layers. It consists of a Fortran-77 program and a VMS DCL command procedure. SPARCOL is used to prepare the X.DAT and X.INN files required by MAIN2 and MAIN2R, and to give these files user-defined names. Although these two files can be created using a text editor, the user may find it helpful to prepare them using SPARCOL.

The MAIN2 program for processing ellipsometric data is documented in NIST Special Publication 400-84, Semiconductor Measurement Technology: A Software Program for Aiding the Analysis of Ellipsometric Measurements, Simple Spectroscopic Models, by J. F. Marchiando, hereafter referred to as the MAIN2 manual [1]. The MAIN2R program is very similar to MAIN2 but has been modified to process reflectance data.

2. LIMITATIONS

There are some limitations of SPARCOL which prevent a user from creating X.DAT and X.INN files to suit all situations. The limitations are:

(a) The ambient is assumed to be air.

(b) The substrate is assumed to have a single constituent as opposed to being a mixture. A constituent may be an element such as silicon or a chemical compound such as silicon dioxide.

(c) Each layer must consist of not more than five constituents.

(d) There must not be more than 40 constituents distributed among the layers. That is, SPARCOL can accommodate 39 layers of one constituent each plus a substrate, 13 layers of three constituents each plus a substrate, or any combination of layers and constituents that does not exceed 40 constituents. This limitation is imposed by array sizes which could be increased.

(e) MAIN2 and MAIN2R provide for passing integer or floating-point parameters to subroutines that calculate the dielectric functions of constituents and mixtures. These supplementary

1

parameters cannot be used with SPARCOL. They are discussed on pages 24, 25, and 67 of the MAIN2 manual.

(f) Only one sample can be processed by a particular X.DAT file.

(g) Command option 1 for plots or forward problem calculation, as described on pages 41 to 45 of the MAIN2 manual, has not been implemented in SPARCOL.

(h) The user must supply a subroutine to convert raw ellipsometric data into the format required by the X.DAT file.

Regarding the last limitation, SPARCOL has within it a CONVRT subroutine which is used in-house at NIST. This CONVRT subroutine can read data in the format generated by a NIST ellipsometer or reflectometer or data which is already in the format required by MAIN2 and MAIN2R. The user must write a replacement for CONVRT to handle data from any other ellipsometer or reflectometer. Further information on data formats is given in section 9.

The comments which appear to the right of the data in example X.DAT and X.INN files in the MAIN2 manual are not generated by SPARCOL. These comments are ignored by MAIN2 and MAIN2R, so their absence does not affect program operation.

3. OVERVIEW

SPARCOL builds the X.DAT and X.INN files from the interactive responses of the user to a series of prompts. The responses to the prompts may be entered in free format.

SPARCOL operates in two phases. In the first phase, the materials or constituents which comprise the various layers are entered. This information can be written to a file which can be read during subsequent analyses of layers having the same constituents. The nature of this layers file is described in section 5.

In the second phase, model parameters such as layer thicknesses, volume fractions of layer constituents, uncertainties, and bounds of search grids are entered. Which parameters are entered depends on whether a layer consists of a single constituent or multiple constituents, and whether the thickness of a layer or the volume fraction of a constituent is being allowed to vary. SPARCOL calculates parameters whenever it can, and it asks only for data which MAIN2 or MAIN2R needs. For example, SPARCOL does not prompt for the volume fraction of the last constituent of a layer because it can be calculated from the fractions previously entered.

The user may pause at any time in phase 2 to examine the data which have been entered so far. The user has the option to re-enter values for the current constituent. This procedure is discussed in section 6.

SPARCOL allows the user to save all the entered model parameters in a file called the array file, so that the parameters can be used with several sets

of ellipsometric or reflectance data without having to re-enter them. The use of the array file is described in section 8.

4. AN EXAMPLE

The following example is based on the worked example which begins on page 61 of the MAIN2 manual as run under the VMS operating system on a DEC VAX computer. It is similar to the first example given in the MAIN2 Quick Reference Guide [2]. The example is simple in that it deals with only a single layer plus transition region, yet it demonstrates a case of practical interest. The example supposes that the thickness of the oxide layer is known and the properties of the transition region are to be calculated. The procedure of the example has been divided into sub-tasks denoted as sections 4.1, 4.2, etc. The computer dialogue is printed in **bold** font. User input is shown underlined.

4.1 SPARCOL Startup--Begin Phase One.

$ SPARCOL DEMO EPX

The first parameter, DEMO, is the filename of the two files that will be created, that is, the X.DAT and X.INN files will be named DEMO.DAT and DEMO.INN. The first letter of the second parameter must be an R if reflectance data are being processed or an E if ellipsometric data are being processed. The R or E must be followed by a P, meaning that X.DAT and X.INN files are to be prepared, an X, meaning that MAIN2 or MAIN2R is to be executed using existing files, or PX, meaning that files are to be prepared then run. There are no defaults.

SPARCOL Program to Create X.DAT and X.INN
files for MAIN2 or MAIN2R.

Enter the information regarding layer
constituent materials by one of the
following methods:

Enter 0 to abort SPARCOL,
1 to use information contained in an existing layers file,
2 to enter information interactively then save to a file,
3 to enter information interactively without saving, or
4 to use SPARCOL information contained in an existing array file.
2

4.2 Create File of Layer Constituents.

Enter the file descriptor of the layers file to be created.
DEMO.LAY

In the most general sense, the file descriptor can consist of a network node name, disk device, directory, filename, extension, and version number. In this example, the layers file is in the user's default directory, so only the filename and extension need to be entered. The filename DEMO is given

3

to most of the example files referred to in this document. The layers file
is not used by MAIN2 or MAIN2R but is a convenient way to store information
used by these programs that does not change from run to run, specifically,
the materials of which the various layers are composed.

How many layers does the sample have,
counting the substrate and all transition
regions as layers?
<u>3</u>

Enter the layer constituents as material numbers. By
convention, layer 1 is the top layer. Enter -1 in
response to the prompt asking for a material number
to display a table of material numbers on the screen.

How many constituents are in layer 1?
<u>1</u>

Enter the material number of the material in layer 1.
<u>-1</u>

Not having the numbers relating to the 17 materials committed to memory,
the user enters -1 to produce the following table. The prompt is then re-
issued. The user may enter -1 again later if the table rolls off the
screen.

```
 1 = Vacuum     2 = Air       3 = Si(Xtal)  4 = Si(Poly)  5 = SiO2
 6 = Si3N4      7 = Ge(Xtal)  8 = GaAs(Xt)  9 = AlGaAs   10 = OxofGaAs
11 = As(Amor)  12 = GaP      13 = GaSb     14 = InAs     15 = InP
16 = InSb      17 = AlSb
```

Enter the material number of the material in layer 1.
<u>5</u>

How many constituents are in layer 2?
<u>2</u>

Enter the material number of material 1 in layer 2.
<u>3</u>

Enter the material number of material 2 in layer 2.
<u>5</u>

Number of constituents of substrate set at 1.

Enter the material number of the material in layer 3.
<u>3</u>

Data entry is now complete and the following table is produced.

The layers file shows the following layers:

```
------------------------------------------------------------------
   Layer    1:  SiO2
------------------------------------------------------------------
   Layer    2:  Si(Xtal) + SiO2
------------------------------------------------------------------
   Layer    3 (Substrate): Si(Xtal)
------------------------------------------------------------------
```

4.3 Verify Layers File (Optional).

Enter 1 to continue or 0 to stop.
<u>0</u>

If the layers in the table are correct, the user can enter 1 above and
proceed to phase 2. For purposes of this example, we enter 0 and take a
look at the layers file.

FORTRAN STOP

SPARCOL aborted.

$ <u>TYPE DEMO.LAY</u>
```
    5
    3   5
    3
```

The layers file is quite simple. The first line contains the number
corresponding to the material in the top layer. The number 5 in the table
above represents silicon dioxide. The second line contains a 3 and a 5,
meaning that the layer contains both crystalline silicon and silicon
dioxide. The 3 in the third line represents the crystalline silicon
substrate. The format of the layers file allows for comments and free
formatting as explained in section 5.

The layers file need not be created by phase 1 of SPARCOL. It can also be
created or modified using a text editor.

We continue with the example. Having already created the DEMO.LAY layers
file, we go directly to phase 2.

5

4.4 Begin Phase Two.

$ <u>SPARCOL DEMO EPX</u>

SPARCOL Program to Create X.DAT and X.INN
files for MAIN2 or MAIN2R.

Enter the information regarding layer
constituent materials by one of the
following methods:

Enter 0 to abort SPARCOL,
      1 to use information contained in an existing layers file,
      2 to enter information interactively then save to a file,
      3 to enter information interactively without saving, or
      4 to use SPARCOL information contained in an existing array file.
 <u>1</u>

When option 1 is selected, SPARCOL asks for the file descriptor of the
layers file. This is the file created previously.

Enter the file descriptor of the layers file.
<u>DEMO.LAY</u>

   3 data records read.
   0 comment records read.
   4 constituents total.

The layers file shows the following levels:

  Layer   1: SiO2

  Layer   2: Si(Xtal) + SiO2

  Layer   3 (Substrate): Si(Xtal)

SPARCOL reports the type of structure being analyzed. SPARCOL could be
aborted at this time if the wrong layers file had been selected. We
continue.

Enter 1 to continue or 0 to stop.
<u>1</u>

The next two questions refer to the type of analysis which is to be
performed on the ellipsometric or reflectance data. Refer to pages 45
through 49 of the MAIN2 manual. If the response to the first question is
"2", then the second question is not asked.

6

4.5   Enter Mode of Execution.

SPARCOL supports two of the MAIN2 program's three modes of execution.
Enter either 2 or 3 to specify which mode is to be used.

   2 - Search   (vary)
   3 - Search grid (vary)

<u>3</u>

There are two options regarding the grid scan.
Enter a 0 or 1 to specify which of these is to be used.

   0 - No optimization, |g| only
   1 - Full optimization, Jacobian

<u>1</u>

4.6   Specify Thickness of Layer 1.

SPARCOL now asks questions about the layer characteristics.

Your layers file indicates that a structure having 3
layers including the Si(Xtal) substrate is to be
analyzed. In the questions that follow, layer 1 is
defined to be the top layer.

Enter -1 for status, to re-enter, or to abort.

The feature that allows the user to see what has been entered so far by
responding with -1 is discussed in section 6. For now, we continue with the
example.

Layer 1 contains SiO2   .

Enter a 1 if the thickness of layer 1 is
to be permitted to vary. Otherwise enter a 0.
<u>0</u>

The question about whether a layer thickness is a variable in the analysis
is always asked first. The answer determines what subsequent questions are
asked. In this example, the thickness of layer 1 is not a variable. If the
thickness is not a variable, the uncertainty is not used, but a value of 0
is supplied and written to the X.DAT file.

Enter the thickness of this layer in nm.
<u>100</u>

Layer 2 contains Si(Xtal) and SiO2   .

Enter a 1 if the thickness of layer 2 is
to be permitted to vary. Otherwise enter a 0.
1

4.7 Specify Thickness of Layer 2.

Unlike layer 1, the thickness of layer 2 is a variable. Because it is a
variable, its value is not requested. A value of 0.00 is written to the
DEMO.DAT file, although MAIN2 and MAIN2R ignore the value. The uncertainty
is entered, however, since that determines the manner in which the analysis
is performed.

Enter the uncertainty of the thickness of
layer 2 in nm.
2.0

Because command option 3 was entered to specify a search grid analysis, the
characteristics of the grid are requested.

Enter the lower bound, upper bound, and step
size in nm for the thickness of this layer.

Lower bound (nm):
1.0

Upper bound (nm):
3.0

Step size (nm):
2.0

4.8 Specify Volume Fraction of Layer 2.

As was the case with layer thickness, the question of whether a particular
constituent's volume fraction is a variable is asked first.

Enter a 1 if the fraction of Si(Xtal) in
layer 2 is to be permitted to vary. Otherwise
enter a 0.
1

Because the volume fraction is a variable, no values of volume fraction are
requested. However, SPARCOL calculates values to place in the DEMO.DAT file
even though these values are ignored by MAIN2 and MAIN2R. The numbers
SPARCOL places represent an even division of the portion of the total volume
fraction still remaining. In this case, each constituent is assigned a
volume fraction of 0.50.

When the volume fraction of one constituent of a layer is permitted to vary,
volume fractions of all subsequent constituents are forced to vary. This is
a constraint imposed by SPARCOL rather than by MAIN2 or MAIN2R. Also, when
volume fractions are permitted to vary, the parameters pertaining to the

8

first varying constituent are ignored by MAIN2 and MAIN2R. Therefore, SPARCOL sets the uncertainty equal to the fraction of the first varying constituent and goes on to the second constituent.

Setting fraction and uncertainty of Si(Xtal) in layer 2 to 0.50

The volume fraction(s) entered so far total 0.50,
so the volume fraction of SiO2   in layer 2 is
being set at 0.50.

Forcing the volume fraction of SiO2   in
layer 2 to vary.

Enter the uncertainty in the volume fraction
of SiO2   in layer 2 expressed as a number
between 0.0 and 1.0.
<u>0.02</u>

As was done with the thickness, enter the bounds relating to the volume fraction of the second constituent of the layer. The last prompt asks for the directory in which the W files are stored. See pages 21 and 296 through 331 of the MAIN2 manual for additional information on the W files.

Enter the lower bound, upper bound, and step
size for the volume fraction of SiO2   in layer 2

Lower bound:
<u>0.3</u>

Upper bound:
<u>0.7</u>

Step size:
<u>0.4</u>

4.9 Locate W. Files.

Enter the device and directory on which the
W. files are stored. Example: DRB1:[DATA_BASES]W.
(The W and the period are required.)
<u>DRB1:[DATA_BASES]W.</u>

4.10 View Model Parameters.

All model parameters have now been entered. SPARCOL produces the display below showing the type of analysis, model parameters, and the location of the W. files.

Analysis: Search grid with full optimization.

Layer #	Element #	Element Name	Thickness, nm	Vary ?	Fraction	Vary ?
1	5	SiO2	100.00 +/- 0.00	0		
2	3	Si(Xtal)	0.00 +/- 2.00	1	0.50 +/- 0.50	1
		Grid:	1.00, 3.00, 2.00			
	5	SiO2			0.50 +/- 0.02	1
					Grid: 0.30, 0.70, 0.40	
3	3	Si(Xtal)	Substrate			

W files located at: DRB1:[DATA_BASES]W.

4.11 Store Model Parameters in Array File.

Having taken the time to enter all these parameters, it is suggested that
they be stored in an array file for later use. The following two prompts
accomplish this. The array file is discussed in section 8.

Enter 1 to store all the model parameters
in an array file. Otherwise enter 0.
1

Enter the file descriptor of the array file to be created.
DEMO.ARR

4.12 Identify Raw Data.

SPARCOL then asks for the type of analysis to be performed and the name of
the raw data file. Each of the four options calls a subroutine to convert
data from a NIST ellipsometer into the format required by MAIN2 or to
convert data from a NIST reflectometer into the format required by MAIN2R.
The user may need to supply a subroutine in place of CONVRT to convert data
into the form required by MAIN2 or MAIN2R. Subroutine CONVRT is discussed
at greater length in section 9.

Specify the type of analysis to be performed.

Enter 1 to process spectroscopic one-zone data
          having multiple wavelengths,
      2 to process single wavelength two-zone
          average data,
      3 to process data already in MAIN2 format, or
      4 to process reflectance data to be run
          on MAIN2R.
3

Enter the file descriptor of the file containing
the raw data from the ellipsometer.
DEMO.RAW

The file DEMO.RAW contains data already in the format required by MAIN2.
The values are given in the example beginning on page 61 of the MAIN2
manual. SPARCOL appends the converted data to the DEMO.DAT file.

All information has now been entered. Because the original SPARCOL command
requested that MAIN2 be executed, it is submitted as a batch job. SPARCOL
then exits.

FORTRAN STOP
Job SPARCOL$DEMO (queue SYS$BATCH, entry nnn) started on SYS$BATCH

SPARCOL run using DEMO.DAT and DEMO.INN has begun.

$

The DEMO.DAT and DEMO.INN files which have been created are shown below.
Values that differ from the values shown on pages 61 and 62 of the MAIN2
manual are indicated by an asterisk. These differences occur only in values
that are ignored by MAIN2, however.

4.13 Examine X.DAT File.

$ TYPE DEMO.DAT
DRB1:[DATA_BASES]W.

 2
    1   100.00   0.00* 0
    2   0.00*   2.00   1

 0

 0

 4
 1   0   0
    1   2   1.00   0.00   0
 1   0   0
    1   3   1.00   0.00   0
 1   0   0
    1   5   1.00   0.00   0
 2   0   0
    1   3   0.50*   0.50*   1
    2   5   0.50*   0.02   1

 1
    1   1   0   0

11

```
   1
   2
    1   3   1
    2   4   2
    3   2
-------------------------------------------------------
   1
   1   1
    10
     1     1.50000E+00   7.00000E+01   8.04309E+01   3.08875E+01
           1.00000E-01   1.00000E-02   1.00000E-02   1.00000E-02
     2     2.00000E+00   7.00000E+01   7.97129E+01   4.31275E+01
           1.00000E-01   1.00000E-02   1.00000E-02   1.00000E-02
     3     2.50000E+00   7.00000E+01   1.02227E+02   6.93018E+01
           1.00000E-01   1.00000E-02   1.00000E-02   1.00000E-02
     4     3.00000E+00   7.00000E+01   2.50415E+02   6.09989E+01
           1.00000E-01   1.00000E-02   1.00000E-02   1.00000E-02
     5     3.50000E+00   7.00000E+01   2.62427E+02   4.00376E+01
           1.00000E-01   1.00000E-02   1.00000E-02   1.00000E-02
     6     4.00000E+00   7.00000E+01   2.47313E+02   3.31054E+01
           1.00000E-01   1.00000E-02   1.00000E-02   1.00000E-02
     7     4.50000E+00   7.00000E+01   1.92800E+02   3.34557E+01
           1.00000E-01   1.00000E-02   1.00000E-02   1.00000E-02
     8     5.00000E+00   7.00000E+01   1.24499E+02   3.21867E+01
           1.00000E-01   1.00000E-02   1.00000E-02   1.00000E-02
     9     5.50000E+00   7.00000E+01   8.77637E+01   3.66717E+01
           1.00000E-01   1.00000E-02   1.00000E-02   1.00000E-02
    10     6.00000E+00   7.00000E+01   7.10687E+01   4.18238E+01
           1.00000E-01   1.00000E-02   1.00000E-02   1.00000E-02
```

4.14   Examine X.INN File.

$ <u>TYPE DEMO.INN</u>
```
   3
    2          1.000         3.000         2.000
    2          0.300         0.700         0.400
    1
```

The DEMO.OUT file produced by MAIN2 agrees with the example on pages 62 to
66 of the MAIN2 manual.

5.   THE LAYERS FILE

In its simplest form, the layers file consists of several lines, the number
of lines being equal to the number of layers in the structure counting the
substrate and all transition regions as layers. Each line contains from one
to five numbers, and each number represents one of 17 materials of which the
layers may consist. More generally, the rules for constructing a layers
file are as follows:

12

(a) Blank lines are ignored.

(b) Lines having no printing characters before a "!" are treated as comments and ignored.

(c) A data line consists of from one to five integers, adjacent integers separated by a delimiter, with the last number optionally followed by a delimiter, exclamation point, and arbitrary comment text. (The exclamation point must be preceded by a delimiter.)

(d) A delimiter consists of any combination of spaces and/or tabs.

(e) The lines cannot be more than 80 characters long.

6. CHECKING STATUS

Within phase 2 of SPARCOL, while entering data regarding layer thicknesses and volume fractions, the user can pause to look at the structure configuration by entering -1 in response to any prompt. As a demonstration, suppose -1 had been entered at the prompt for the upper bound of the thickness of layer 2 in the previous example.

Upper bound (nm):
<u>-1</u>

Enter 0 to abort the program,
     1 to display the data entered so far,
     2 to display levels and constituents,
     3 to return to the previous data input prompt, or
     4 to re-enter all data for the current constituent.
<u>2</u>

Entering -1 calls up a menu having five options. Option 2 produces a display of the levels and constituents which comprise the structure. This is the same display which appeared in phase 1 of SPARCOL. Following the display, the menu appears again.

The input file shows the following levels:

```
----------------------------------------------------------------
  Layer   1:  SiO2
----------------------------------------------------------------
  Layer   2:  Si(Xtal) + SiO2
----------------------------------------------------------------
  Layer   3 (Substrate): Si(Xtal)
----------------------------------------------------------------
```

13

Enter 0 to abort the program,
      1 to display the data entered so far,
      2 to display levels and constituents,
      3 to return to the previous data input prompt, or
      4 to re-enter all data for the current constituent.
1

Option 1 produces a table of all the data entered thus far. Note that a -1
appears in the table at the point of the current prompt. (It is possible to
produce multiple -1's in the table by electing to re-enter all data for the
current constituent, then responding again to a data input prompt with -1.)
Analysis: Search grid with full optimization.

Layer #	Element #	Element Name	Thickness, nm	Vary ?	Fraction	Vary ?
1	5	SiO2	100.00 +/- 0.00	0		
2	3	Si(Xtal)	0.00 +/- 2.00	1	0.00 +/- 0.00	0
		Grid:	1.00, -1.00, 0.00			

Enter 0 to abort the program,
      1 to display the data entered so far,
      2 to display levels and constituents,
      3 to return to the previous data input prompt, or
      4 to re-enter all data for the current constituent.

You can go back to the prompt from which you came by entering option 3.
Alternatively, option 4 can be used to re-enter all data pertaining to the
current constituent. Entering 0 aborts SPARCOL.

7. OMITTING A LAYER

There may be times when a layers file has been created which defines a
structure, and the user wants to remove one of the layers in the structure.
The user could create a new layers file, but it is not necessary. The user
needs only to respond with 0 to the vary flag and thickness prompts for that
layer. SPARCOL will automatically remove that layer and renumber the layers
as needed. Multiple layers can be removed. SPARCOL makes no judgment
regarding whether removal of layers constitutes a realistic situation.

As a demonstration, the previous example is run with the transition region,
layer 2, removed. Some of the computer dialogue has been edited out as
indicated by ellipses.

$ SPARCOL DEMO EPX
 . . .
Enter the file descriptor of the layers file.
DEMO.LAY
 . . .

The input file shows the following levels:

```
---------------------------------------------------------------
  Layer   1:  SiO2
---------------------------------------------------------------
  Layer   2:  Si(Xtal) + SiO2
---------------------------------------------------------------
  Layer   3 (Substrate): Si(Xtal)
---------------------------------------------------------------
```

. . .

Layer 1 contains SiO2   .

Enter a 1 if the thickness of layer 1 is
to be permitted to vary. Otherwise enter a 0.
<u>0</u>

Enter the thickness of this layer in nm.
<u>100</u>

Layer 2 contains Si(Xtal) and SiO2   .

Enter a 1 if the thickness of layer 2 is
to be permitted to vary. Otherwise enter a 0.
<u>0</u>

Enter the thickness of this layer in nm.
<u>0</u>

Enter the device and directory on which the
W. files are stored. Example: DRB1:[DATA_BASES]W.
(The W and the period are required.)
<u>DRB1:[DATA_BASES]W.</u>

Note: 1 zero-thickness layer(s) containing
       2 constituent(s) has been removed.

Analysis: Search grid with full optimization.

Layer #	Element #	Element Name	Thickness, nm	Vary ?	Fraction	Vary ?
1	5	SiO2	100.00 +/- 0.00	0	.	
2	3	Si(Xtal)	Substrate			

W files located at: DRB1:[DATA_BASES]W.

The transition region has been removed and the layers renumbered. A
message appears above the table to indicate that a layer has been removed.
Note, however, that there are no longer any varying model parameters to be
calculated, an unrealistic situation.

8. THE ARRAY FILE

In the example of section 4, an array file was created. The array file contains a value indicating the type of analysis to be performed, all the model parameters, and the device and directory containing the W files. The array file takes its name from the IARRAY and RARRAY arrays which contain the values of all the model parameters. It is primarily these two arrays that are written to the array file. Some information on these arrays is given in the initial comments of the SPARCOL.FOR program.

The array file can be read back using option 4 of the menu which comes up when SPARCOL is first run. This is useful when several sets of ellipsometric or reflectance data are to be processed using the same model parameters. (MAIN2 and MAIN2R provide for processing multiple data sets, but this feature is not directly built into SPARCOL.) The following example shows how the DEMO.ARR file can be read by SPARCOL.

$ <u>SPARCOL DEMO EPX</u>
```
. . .
```
Enter 0 to abort SPARCOL,
      1 to use constituent information contained in an existing layers file,
      2 to enter information interactively then save to a layers file,
      3 to enter information interactively without saving, or
      4 to use SPARCOL information contained in an existing array file.
<u>4</u>

Enter the file descriptor of the array file.
<u>DEMO.ARR</u>

Analysis: Search grid with full optimization.

Layer #	Element #	Element Name	Thickness, nm	Vary ?	Fraction	Vary ?
1	5	SiO2	100.00 +/- 0.00	0		
2	3	Si(Xtal)	0.00 +/- 2.00	1	0.50 +/- 0.50	1
		Grid: 1.00, 3.00,	2.00			
	5	SiO2			0.50 +/- 0.02	1
					Grid: 0.30, 0.70, 0.40	
3	3	Si(Xtal)	Substrate			

W files located at: DRB1:[DATA_BASES]W.

```
. . .
```
FORTRAN STOP

9. SUBROUTINE CONVRT

The CONVRT subroutine supplied with SPARCOL enables ellipsometric or

reflectance data to be read and incorporated into the X.DAT file. The four
options appear in the prompting message shown in section 4.12 above. The
first two options involve subroutines CONV1 and CONV2. These relate to a
NIST ellipsometer, a unique instrument whose data format is of interest
primarily to NIST staff. The third choice uses subroutine CONV3 to accept
data that have already been converted to the format required by MAIN2 by
means of a separate, user-written preprocessing program. The fourth choice
uses subroutine CONV4 to read a file of wavelength-reflectance pairs, where
the first line of the file is skipped, wavelengths are in nanometers, and
reflectance is expressed as a number between 0 and 1.

The user must either write a subroutine to replace CONV1, CONV2, or CONV4,
or write a preprocessor and then use option 3. The example which has been
used in this document is preprocessed data read by option 3. The actual
data appear on page 38 of the MAIN2 manual. On that page, the output of
CONVRT begins on the fourth line, the row of dashes being the first line.
CONVRT generates the line containing the number of measurements and two
lines for every measurement after that. The example uses E format, but F
format also works. The indices must be INTEGER type. Comments and
parenthetical text that appear in the MAIN2 manual are not needed by MAIN2
or MAIN2R and have been omitted.

10. ERROR CHECKING

SPARCOL does some checking of data entered interactively or contained in the
layers file. Following are the error messages which SPARCOL produces. In
some cases, the error message may occupy more than one line, even though
printed on a single line below.

Each of the four letters (R,E,P,X) can appear only once. The second
parameter of the SPARCOL command may not have repeated characters.

Either <file>.DAT or <file>.INN was not found. One or both of the files
needed by MAIN2 or MAIN2R cannot be found.

Either R or E, and either P or X must appear in the second parameter. There
are no defaults in the SPARCOL command line. Either R or E and either P or
X (or both) must appear in the second parameter of the command line.

Element number i has already been entered as a constituent of this layer.
An element number cannot be repeated in any given line of the layers file.

Element numbers must be in the range 1 to 17 inclusive. Only the integers 1
through 17 have been assigned corresponding materials. Other numbers have
no meaning.

Error reading array file. The array file is not in the proper format.

Exiting from SPARCOL.COM due to error condition. An error other than those
explicitly provided for has occurred in the SPARCOL.COM command procedure.
This could be caused, for example, by attempting to create the X.DAT and
X.INN files in a directory to which the user does not have write access.

17

File not found -- Reprompt. The file containing the ellipsometric data could not be found. This message originates in subroutine CONVRT, and so could change when the user supplies an equivalent routine.

File not found -- returning to menu. Indicates that the layers file or array file specified after entering option 1 or 4 in the menu of phase 1 cannot be found.

Illegal character X in position i of record n of <file>. A non-numeric character which is not preceded by an exclamation point has been encountered in the layers file.

Illegal negative value, or lower > upper. Unallowed values have been entered for the range of variation of the layer thickness.

Number of constituents exceeds 40. Re-dimension arrays and make other program changes. SPARCOL was written to handle only 40 constituents. The program will need to be modified to accommodate more.

Number of constituents must be in the range 1 to 5 inclusive. A layer can have from one to five constituents.

Number of layers must be greater than 1. The number of layers in the structure must be greater than 1, because the substrate counts as a layer.

R and E cannot both appear in the second parameter. The SPARCOL command must indicate unambiguously whether ellipsometric or reflectance data are to be processed.

Repeated constituent in record n of <file>. The same integer appears more than once in a single record of the layers file.

Substrate (last line in input file) must consist of only one constituent. The last record of the layers file can contain only one integer.

Sum of fractions is > 1.5 or < -0.5. This message appears after the fractions of all constituents except the last have been entered. SPARCOL has summed the fractions and realizes that the fraction for the remaining constituent cannot be assigned a legal value that will cause the sum of the fractions to be 1.0 as required.

The command must have EXACTLY two parameters following it. The SPARCOL command must be followed by two arguments.

The letter <letter> is not allowed -- Exiting. Only the letters R, E, P, and X can appear in the second argument to the SPARCOL command.

There are more than the maximum of 5 integers in record n of <file>. The entries in the layers file cannot specify more than five constituents in any layer.

Unable to create JOBFILE, possibly due to directory protection. SPARCOL must be run in a directory to which the user has write access so that JOBFILE (the batch run stream) can be created.

Uncertainty must be in the range 0.0 to 1.0. The uncertainty of the volume fraction must be in the range 0 to 1.

Value must be a 0 or a 1. The vary flag for thicknesses and fractions can only be 0 or 1.

Value outside of range -0.5 to 1.5, upper bound < lower bound, or step size < 0. Unallowed values have been entered for the range of variation of the volume fraction of constituents of a layer.

Values greater than 1.5 or less than -0.5 are not allowed. The values of fraction for an individual constituent are limited to the range 1.5 to -0.5 inclusive.

11. PORTABILITY, AVAILABILITY, AND INSTALLATION

SPARCOL consists of SPARCOL.FOR, written in FORTRAN-77, and SPARCOL.COM, a VMS DCL command procedure. SPARCOL.FOR compiles and runs under VMS 5.3-1 and SunOS 3.5. The example of section 4 runs successfully on both of these platforms. On non-VMS machines, the DCL command procedure does not work, but the SPARCOL executable can be run, and files can be renamed and jobs can be submitted manually. It is assumed that SPARCOL could be ported to other computing environments as well. The MAIN2 program was written to run under VMS [3], but a version that runs under SunOS 3.5 is also available. The SunOS version of MAIN2 does not do file checkpointing or report execution time.

The source code and accompanying files are available on three media: (1) on half-inch tape at 800 or 1600 bpi, in DEC Files-11 format, written by the VMS COPY command, (2) on 5.25-in., 360-KB diskette, and (3) on 3.5-in. 1.44-MB diskette. When supplied on diskette, this report is included in WordPerfect 5.0 format. To request this software, contact Richard L. Mattis, Semiconductor Electronics Division, National Institute of Standards and Technology, Gaithersburg, Maryland 20899.

The following files are supplied:

    SPARCOL.COM, the VMS DCL command procedure.
    SPARCOL.FOR, the FORTRAN-77 source code.
    SPARCOL.DOC, this document in plain ASCII format.
    SPARCOL.WP, this document in WordPerfect 5.0 format.
    EXAMPLE.LAY, the DEMO.LAY file created in section 4.
    EXAMPLE.DAT, the DEMO.DAT file created in section 4.
    EXAMPLE.INN, the DEMO.INN file created in section 4.
    EXAMPLE.ARR, the DEMO.ARR file created in section 4.

To install SPARCOL on a VAX/VMS system, create a suitable directory if one does not already exist, and copy the files from the tape into that

19

directory. The commands would be similar to the following, where the underlines used previously have been omitted.

```
$ CREATE/DIR dev:[directory]
$ SET DEF dev:[directory]
$ ALLOCATE MTA0:
$ MOUNT/NOWRITE MTA0: NIST
$ COPY MTA0:*.* []
$ DISMOUNT MTA0:
$ DEALLOCATE MTA0:
$ FORTRAN SPARCOL
$ LINK SPARCOL
```

The following symbol must be defined before SPARCOL is run. This command line can be typed by the user, placed in the user's LOGIN.COM file, or placed in the SYS$MANAGER:SYLOGIN.COM file.

```
$ SPARCOL := @dev:[directory]SPARCOL
```

When the files are supplied on an MS-DOS diskette, the files must be transferred to a VAX/VMS or Sun system using a file transfer program such as Kermit, DECNET, or FTP. Once that is done, the SPARCOL.FOR file need only be compiled and linked as given above.

12. ACKNOWLEDGMENTS

The author is indebted to Jay F. Marchiando, without whose help in understanding MAIN2 the SPARCOL program could not have been written, to Barbara J. Belzer for careful critiques of this document with an eye to the user, and to Jon C. Geist for helpful discussions which clarified the objectives and focus of the program.

13. REFERENCES

[1] Marchiando, J. F., Semiconductor Measurement Technology: A Software Program for Aiding the Analysis of Ellipsometric Measurements, Simple Spectroscopic Models, NIST Special Publication 400-84, April 1990.

[2] Marchiando, J. F., Quick Reference Guide for NIST Special Publication 400-84, June 1990.

[3] Marchiando, J. F., Installation Guide for NIST Special Publication 400-84, June 1990.

4. TITLE AND SUBTITLE

SPARCOL: A Front End for the MAIN2 Program

5. AUTHOR(S)

Richard L. Mattis

11. ABSTRACT (A 200-WORD OR LESS FACTUAL SUMMARY OF MOST SIGNIFICANT INFORMATION. IF DOCUMENT INCLUDES A SIGNIFICANT BIBLIOGRAPHY OR LITERATURE SURVEY, MENTION IT HERE.)

SPARCOL is an interactive program which serves as a front-end to the MAIN2 and MAIN2R computer programs. SPARCOL (pronounced "sparkle") stands for SPectroscopic ellipsometry And Reflectance for Characterization Of Layers. It consists of a Fortran-77 program and a VMS DCL command procedure. SPARCOL is used to prepare the X.DAT and X.INN files required by MAIN2 and MAIN2R, and to give these files user-defined names. Although these two files can be created using a text editor, the user may find it helpful to prepare them using SPARCOL.

The MAIN2 program for processing ellipsometric data is documented in NIST Special Publication 400-84, Semiconductor Measurement Technology: A Software Program for Aiding the Analysis of Ellipsometric Measurements, Simple Spectroscopic Models, by J. R. Marchiando, referred to in the publication as the MAIN2 manual. The MAIN2R program is very similar to MAIN2 but has been modified to process reflectance data.

12. KEY WORDS (6 TO 12 ENTRIES; ALPHABETICAL ORDER; CAPITALIZE ONLY PROPER NAMES; AND SEPARATE KEY WORDS BY SEMICOLONS)

ellipsometry; EMA; FORTRAN; layer thickness; modeling; reflectance; spectroscopic models