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NIST
PUBLICATIONS

NISTIR 4969

MAESTRO: A Front-End to the MAIN1 Program for Multiple-Angle Measurement of Silicon Dioxide Layers

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December 1992

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MAESTRO: A Front-End to the MAIN1 Program for Multiple-Angle Measurement of Silicon Dioxide Layers

by

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ABSTRACT

MAESTRO is an interactive program which serves as a front-end to the MAIN1 computer program for processing ellipsometric data. It is applicable when MAIN1 is used to characterize silicon dioxide layers on silicon substrates using a single pair of Delta-psi values, using repeated pairs of Delta-psi values taken at the same nominal angle of incidence, or using pairs of Delta-psi values taken at multiple angles of incidence. MAESTRO stands for Multiple-Angle Ellipsometry for Supplying Thickness and Refractive index Output. It consists of two FORTRAN programs and a VMS DCL command procedure. An implementation for MS-DOS is also available. MAESTRO is used to prepare the X.DAT file required by MAIN1 and to give this file and the MAIN1 output files user-defined names.

Key words: ellipsometry; FORTRAN; index of refraction; layer thickness; modeling; standards.

1. INTRODUCTION

MAESTRO, for Multiple-Angle Ellipsometry for Supplying Thickness and Refractive index Output, is an interactive computer program which serves as a front-end to the MAIN1 computer program for processing ellipsometric data. It is applicable when MAIN1 is used to characterize silicon dioxide layers on silicon substrates using a single pair of Delta-psi values, using repeated pairs of Delta-psi values taken at the same nominal angle of incidence, or using pairs of Delta-psi values taken at multiple angles of incidence. For repeated pairs or pairs representing multiple angles of incidence, a composite value of oxide thickness is calculated. The original MAESTRO was written to run under VAX/VMS, but a version which runs under MS-DOS on a computer having a 386 processor is also available.[1] Parenthetical paragraphs describe the MS-DOS version where it differs significantly from the VAX/VMS version.

---

[1]Certain commercial equipment, instruments, software codes, or materials are identified in this paper in order to specify adequately the experimental procedure. Such identification does not imply recommendation or endorsement by the National Institute of Standards and Technology, nor does it imply that the materials or equipment identified are necessarily the best available for the purpose.

The MAIN1 program for processing ellipsometric data is documented in NIST Special Publication 400-83, Semiconductor Measurement Technology: A Software Program for Aiding the Analysis of Ellipsometric Measurements, Simple Models, by J. F. Marchiando [1]. Whereas MAESTRO is limited to characterizing silicon dioxide on silicon, in general MAIN1 can calculate layer thicknesses of a variety of layered structures.

MAESTRO prepares a data file called X.DAT which MAIN1 uses to calculate the oxide layer thickness of a collection of samples, which can have different nominal layer thicknesses, and a collective best value for the thickness of the interfacial layer (hereafter called the interlayer) at the silicon-silicon dioxide boundary. Alternatively, the calculation can be run assuming there is no interlayer.

MAESTRO consists of three programs. The first program, written in FORTRAN, is MAESTRO.FOR. Here the user inputs the model parameters such as light wavelength, index of refraction of silicon, and so on. The user indicates which model parameters are fixed and which are to be calculated by MAIN1. The second program, also written in FORTRAN, is STOF.FOR. It produces a summary, contained in the file X.RES, of the output of MAIN1 that is extracted from the longer X.OUT file. The third program is MAESTRO.COM, written in DCL, the VMS command language. It passes filenames from its command line to MAESTRO.FOR and STOF.FOR, makes sure that needed files exist, and decides whether input files to MAIN1 are to be prepared, MAIN1 is to be executed, or both. It also cleans up temporary files when the process is complete.

The MAIN1 program takes an input file X.DAT and produces an output file X.OUT. MAESTRO allows the user to substitute other filenames for X.DAT, X.OUT, etc. while keeping the file extensions. This document sometimes refers to the X.DAT, X.OUT, or other X. files as generic file types which would have other filenames assigned by the user.

(The three parts of the MS-DOS version of MAESTRO are MAESDOS.FOR, STOF2.FOR, and MAESTRO.BAT. The two FORTRAN programs and the MS-DOS version of MAIN1.FOR were compiled using the University of Salford FTN77/386 compiler. A Salford run-time library must be loaded for the corresponding FORTRAN executables to run.[2] MAESTRO.BAT is an MS-DOS command procedure. In the examples that follow, the MS-DOS "C>" prompt would replace that VMS "$" prompt. "TYPE" is both a VMS and an MS-DOS command.)

2. THE MODEL PARAMETER FILE

Before using MAESTRO to prepare an X.DAT file for MAIN1, you must first create a file of the model parameters which are used in the calculation. This file can be created using a text editor. An example is given below. The lines containing the numerical values must be in the order given. The descriptions which follow the numerical values are optional. In these descriptions, n and

[2] The library is supplied with the compiler but may be purchased separately. For information regarding this software, contact OTG Systems, Inc. of Clifford, Penna.

k refer to the real and imaginary parts of the index of refraction. Comment lines, the ones beginning with "!" in the first character position, can be inserted anywhere. The computer dialogue is printed in **bold** font. User input is shown underlined.

```
$ TYPE PARAMS.FIL

!
! Sample PARAMS.FIL file.
!
! Any line beginning with a "!" is ignored.
!
632.8       Incident light wavelength, lambda, nm
1.00027     n of air
!
! Properties of silicon.
!
3.875       n of silicon
0.000       uncertainty of n of silicon
0           1 if n of silicon is allowed to vary; else 0
!
0.0156      k of silicon
0.000       uncertainty of k of silicon
0           1 if k of silicon is allowed to vary; else 0
!
! Properties of silicon dioxide.
!
1.461       n of silicon dioxide
0.002       uncertainty of n of silicon dioxide
1           1 if n of silicon dioxide is allowed to vary; else 0
!
0.000       k of silicon dioxide
0.000       uncertainty of k of silicon dioxide
0           1 if k of silicon dioxide is allowed to vary; else 0
!
! Properties of the interlayer.
!
2.8         n of the interlayer
0.002       uncertainty of n of the interlayer
1           1 if n of the interlayer is allowed to vary; else 0
!
0.000       k of the interlayer
0.000       uncertainty of k of the interlayer
0           1 if k of the interlayer is allowed to vary; else 0
!
1.000       thickness of the interlayer in nm
0.500       uncertainty of the thickness of the interlayer in nm
1           1 if the thickness of the interlayer is allowed to vary; else 0 !
! End of PARAMS.FIL
```

3. ELLIPSOMETRIC DATA FILES

MAESTRO allows the ellipsometric data to be contained in as many as 50 files, but each file must contain data from wafers having the same nominal oxide layer thickness. Within these files, collectively there may be up to 150 sets of ellipsometric data. This limit may be increased by appropriate changes in the array sizes specified in MAESTRO.FOR and the DEFNIT. file of MAIN1.

MAESTRO recognizes repeated or multiple-angle measurements by examining the measurement descriptors contained in the odd-numbered lines of the data files. These measurement descriptors are up to 30 characters long (e.g., TEST #1431), assigned by the user. They may be just a sample number or they may contain additional information. Repetition of the same measurement descriptor indicates data from the same wafer taken at multiple angles. A change in measurement descriptor signals the start of data for a new thickness calculation. Note that a difference in upper case vs. lower case is considered a change in the measurement descriptor, but a change in the number of trailing spaces following the measurement descriptor is not.

Measurement values are contained in the even-numbered lines of the file. The six values from left to right are: angle of incidence phi, ϕ, in degrees, uncertainty in ϕ or $\delta\phi$, the polarization angle Delta, Δ, in degrees, uncertainty in Δ or $\delta\Delta$, the polarization angle psi, ψ, and the uncertainty in ψ or $\delta\psi$.

In the example which is presented in section 4, the data are contained in two files: TEST50.DAT and TEST100.DAT, which are from wafers having nominal oxide layer thicknesses of 50 and 100 nm. The contents of these two files are given below. Note that the first file contains five sets of data with the same measurement descriptor. These are actually five repetitions of data taken from the same sample. MAIN1 will calculate a single composite value of layer thickness from these five sets of data.

In the second file, the first three data sets are processed together as are the last two data sets.

```
$ TYPE TEST50.DAT
TEST #1431
     69.997      0.002    94.38      0.00      23.37     0.00
TEST #1431
     70.00      0.002    93.82      0.00      23.43     0.00
TEST #1431
     70.850     0.002       90.29     0.01         23.34     0.00
TEST #1431
     70.85      0.002       89.77     0.01         23.39     0.00
TEST #1431
     70.890     0.002       90.06     0.01         23.34     0.00

$ TYPE TEST100.DAT
TEST #1323  nist
     69.997     0.002     79.09      0.00     41.96     0.00
```

```
TEST #1323  nist
     67.200      0.002      89.44      0.01     42.24     0.00
TEST #1323  nist
     67.030      0.002      90.09      0.00     42.28     0.00
TEST #1323  test
     70.00       0.002      90.858     0.00     41.978    0.00
TEST #1323  test
     67.20       0.002      89.29      0.01     42.25     0.00
```

The two file specifiers and the nominal oxide-layer thickness represented by the data in each file can be entered interactively in MAESTRO. Alternatively, a file can be created before MAESTRO is initiated which contains this information, as in the example that is shown below. The two file specifiers and the respective nominal oxide thicknesses are contained in the file TEST.FLS.

```
$ TYPE TEST.FLS
TEST50.DAT   50
TEST100.DAT 100
```

4. AN EXAMPLE

4.1 Starting MAESTRO

The MAESTRO.COM file as distributed by NIST contains three directory names and one queue name which need to be changed to suit the user's operating environment. The three directory names each follow a RUN command and can be located using an editor and searching for "$ RUN". The queue name follows the string "QUEUE=" and can be similarly located and changed using an editor.

Set the default directory to the directory containing your files. Define the MAESTRO symbol if this has not already been done in your LOGIN.COM file. In this example, the default directory is [DIR1], and MAESTRO and other program files are in directory [DIR2].

```
$ SET DEF [DIR1]
$ MAESTRO :== @[DIR2]MAESTRO
```

The MAESTRO command allows you to prepare an X.DAT file, execute MAIN1 using an X.DAT file already prepared, or both prepare and execute, depending on whether the last argument of MAESTRO is P, X, or PX (or XP). The first argument of MAESTRO is the filename of the X.DAT file to be used. A .DAT extension is assumed. If the X.OUT file produced by MAIN1 is to have a different filename from the X.DAT file, that filename should follow the name of the input file. In the example below, the output file of MAIN1 will have the same name as its input file.

```
$ MAESTRO TEST PX
```

(The MAESTRO command for MS-DOS works the same way. Use chdir or cd to set the default directory to the directory containing your files. Make sure the

directory or directories containing MAESTRO.BAT, MAESDOS.EXE, and STOF2.EXE are in the path before typing MAESTRO at the "C>" prompt.)

The first prompt asks us to supply the file specifier of a file containing the model parameters.

Enter the file specifier of the file containing the model parameters.
PARAMS.FIL

4.2 Examining the Model Parameters

The menu below then appears. If we are sure that the model parameters in PARAMS.FIL are correct, we can select option 1 from the menu and proceed. Instead we opt to look at the model parameters by selecting option 2.

```
Type 0 to EXIT
     1 to generate X.DAT from the current model parameters
     2 to view the current model parameters
     3 to modify the current model parameters
2
```

```
The current model parameters have the following values:

Wavelength = 632.800        n of air = 1.00027

Silicon model parameters:

n of Si     = 3.8750,  unc. = 0.0000,  vary (1/0) = 0
k of Si     = 0.0156,  unc. = 0.0000,  vary (1/0) = 0

Silicon dioxide model parameters:

n of SiO2   = 1.4610,  unc. = 0.0020,  vary (1/0) = 1
k of SiO2   = 0.0000,  unc. = 0.0000,  vary (1/0) = 0

Interlayer model parameters:

n of ilayer = 2.8000,  unc. = 0.0020,  vary (1/0) = 1
k of ilayer = 0.0000,  unc. = 0.0000,  vary (1/0) = 0
thickns, nm = 1.0000,  unc. = 0.5000,  vary (1/0) = 1

Press RETURN to continue . . .
```

4.3 Altering the Model Parameters

For the purpose of this example, assume that we want to change two model parameters. We enter option 3 when the menu reappears, then follow instructions to make corrections.

```
Type 0 to EXIT
     1 to generate X.DAT from the current model parameters
```

```
     2 to view the current model parameters
     3 to modify the current model parameters
3

Type in new values in response to the following
  prompts.  Press RETURN to keep old values.

Wavelength, nm = 632.800                         >
n of air = 1.00027                               >
n of silicon = 3.8750                            >
Unc. of n of silicon = 0.0000                    >
Vary flag for n of silicon = 0                   >
k of silicon = 0.0156                            >
Unc. of k of silicon = 0.0000                    >
Vary flag for k of silicon = 0                   >
n of SiO2 = 1.4610                               > 1.462
n of SiO2 changed from 1.4610 to 1.4620

Unc. of n of SiO2 = 0.0020                       >
Vary flag for n of SiO2 = 1                      > 0
Vary flag for n of SiO2 changed from 1 to 0

k of SiO2 = 0.0000                               >
Unc. of k of SiO2 = 0.0000                       >
Vary flag for k of silicon = 0                   >
n of interlayer = 2.8000                         >
Unc. of n of interlayer = 0.0020                 >
Vary flag for n of interlayer = 1                >
k of interlayer = 0.0000                         >
Unc. of k of interlayer = 0.0000                 >
Vary flag for k of interlayer = 0                >
Thickness of interlayer, nm = 1.0000             >
Unc. of thickness of interlayer = 0.5            >
Vary flag for thickness of interlayer = 1        >

Type 0 to EXIT
     1 to generate X.DAT from the current model parameters
     2 to view the current model parameters
     3 to modify the current model parameters
     4 to write altered model parameters to a new file
```

4.4 Saving the Altered Model Parameters

We have changed two model parameters. Notice that an option 4 now appears in the menu in addition to the options we saw previously. We may write out the altered parameters to a file which can be read by MAESTRO in a later run. This is shown below.

```
4

Enter the file descriptor of the parameter file to be created.
PARAMS.MOD
```

This creates the file PARAMS.MOD.

(In the MS-DOS version, if a file by that name already exists, a message appears asking the user whether or not MAESTRO should overwrite that existing file. The user may answer 'Y' to overwrite or 'N' to be prompted for another file descriptor.)

4.5 A Last Check on the Model Parameters

It is not possible to view the PARAMS.MOD file from within MAESTRO, but the user can view the current model parameters by requesting menu option 2 again as is done below. Note also that option 4 has disappeared from the menu. MAESTRO presents the option to write a new model parameter file only when model parameters differ from the latest model parameter file.

```
Type 0 to EXIT
     1 to generate X.DAT from the current model parameters
     2 to view the current model parameters
     3 to modify the current model parameters
2
The current model parameters have the following values:

Wavelength = 632.800        n of air = 1.00027

Silicon model parameters:

n of Si      = 3.8750,  unc. = 0.0000,  vary (1/0) = 0
k of Si      = 0.0156,  unc. = 0.0000,  vary (1/0) = 0

Silicon dioxide model parameters:

n of SiO2    = 1.4620,  unc. = 0.0020,  vary (1/0) = 0
k of SiO2    = 0.0000,  unc. = 0.0000,  vary (1/0) = 0

Interlayer model parameters:

n of ilayer = 2.8000,  unc. = 0.0020,  vary (1/0) = 1
k of ilayer = 0.0000,  unc. = 0.0000,  vary (1/0) = 0
thickns, nm = 1.0000,  unc. = 0.5000,  vary (1/0) = 1

Press RETURN to continue . . .

Type 0 to EXIT
     1 to generate X.DAT from the current model parameters
     2 to view the current model parameters
     3 to modify the current model parameters
1
```

4.6 Identifying the Ellipsometric Data Files

We have decided that our model parameters are properly set, and it is time to proceed. The next menu allows us to specify the ellipsometric data in one of

two ways. This was discussed above in section 3. In this example we use the TEST.FLS file.

```
Type 1 to enter the file specifiers and nominal
       oxide thicknesses interactively, or
     2 to enter the file specifier of a file
       containing this information.
2
Enter file specifier of file containing data
  file specifiers and nominal thicknesses.
TEST.FLS
FORTRAN STOP
```

At this point, the MAESTRO FORTRAN program completes. The X.DAT file has been created. Files X.NAM and X.PRM are also produced and are described below. Because the last argument to MAESTRO was PX (see section 4.1), MAESTRO executes MAIN1 using the prepared file. A job file is created and submitted to the system batch queue. Messages indicate that the job has started.

```
Job MAESTRO$TEST (queue SYS$BATCH entry 227) started on SYS$BATCH

MAESTRO run using TEST.DAT has begun.

Job MAESTRO$TEST (queue SYS$BATCH entry 227) completed
```

(In the MS-DOS version, MAIN1 executes within the MAESTRO.BAT file rather than being run in a VMS batch queue. There is no queued job facility in MS-DOS. The listing of MAESTRO$TEST.COM below therefore has no MS-DOS counterpart.)

5. MAESTRO OUTPUTS

The job has completed. Look at the job file which MAESTRO created. Note that the device name, dev:, and the directory names are site-specific.

```
$ TYPE MAESTRO$TEST.COM
$ SET DEFAULT dev:[DIR1]
$ COPY TEST.DAT X.DAT
$ RUN dev:[DIR2]MAIN1
$ RENAME X.OUT TEST.OUT
$ RENAME X.PLOT TEST.PLOT
$ ASSIGN/USER TEST.OUT FOR011
$ ASSIGN/USER TEST.RES FOR012
$ ASSIGN/USER TEST.NAM FOR014
$ RUN [DIR2]STOF
$ EXIT
```

Following is the X.DAT file which MAESTRO produced.

```
$ TYPE TEST.DAT

   2
   1
```

```
1      632.800
1
1       1.00027
6
1     3.8750      0.0000    0
2     0.0156      0.0000    0
3     1.4620      0.0020    0
4     0.0000      0.0000    0
5     2.8000      0.0020    1
6     0.0000      0.0000    0
 4
 1       1.0000      0.5000    1
 2      50.0000      0.5000    1
 3     100.0000      0.5000    1
 4     100.0000      0.5000    1
 3
1     2     1
1     1
1     3     4     2
2     5     6     1
3     1     2
1     1
2     2     1
1     1
1     3     4     3
2     5     6     1
3     1     2
1     1
3     2     1
1     1
1     3     4     4
2     5     6     1
3     1     2
1     1
  5     1     1        TEST #1431
1       69.997      0.002        94.38       0.00       23.37       0.00
2       70.00       0.002        93.82       0.00       23.43       0.00
3       70.850      0.002        90.29       0.01       23.34       0.00
4       70.85       0.002        89.77       0.01       23.39       0.00
5       70.890      0.002        90.06       0.01       23.34       0.00
  3     1     1        TEST #1323  nist
1       69.997      0.002        79.09       0.00       41.96       0.00
2       67.200      0.002        89.44       0.01       42.24       0.00
3       67.030      0.002        90.09       0.00       42.28       0.00
  2     1     1        TEST #1323  test
1       70.00       0.002        78.858      0.00       41.978      0.00
2       67.20       0.002        89.29       0.01       42.25       0.00
```

Note that the file TEST50.DAT was found to contain data for a single sample measured at five angles, and the file TEST100.DAT was found to contain data for two samples based on the two measurement descriptors.

Following is the X.OUT file which MAIN1 produced. Some lines have been truncated on the right or compressed because they are intended for 132-column printout and extend beyond the edge of the page.

```
$ TYPE TEST.OUT
 options:    1,  forward problems, plots, ...
             2,  search        (     vary)
             3,  search grid   (     vary)
             4,  search grid   (froz,vary)
             5,  sensitivity analysis
             6,  MAE plots ~ uncertainty

 Enter:    option ~
           option ~ 2

 mwaves =    1, number of distinct wavelengths
             1     632.8000

 mbient =    1, number of distinct ambient environments and waves.
             1     1.000270

 mlmnts =    6, number of distinct:    n+ik
             1       3.8750       0.0000     0
             2       0.0156       0.0000     0
             3       1.4620       0.0020     0
             4       0.0000       0.0000     0
             5       2.8000       0.0020     1
             6       0.0000       0.0000     0

 mfilmm =    4, number of distinct film widths
             1       1.0000       0.5000     1
             2      50.0000       0.5000     1
             3     100.0000       0.5000     1
             4     100.0000       0.5000     1

 msampl =    3, number of distinct samples
             1   2   1         ~ sample, mfilm, mwave
             1   1             ~ iwave, mbien
             1   3   4   2     ~ i,n,k,z
             2   5   6   1     ~ i,n,k,z
             3   1   2         ~ i,n,k
             1   1             ~ imbien, mrpeat

             2   2   1         ~ sample, mfilm, mwave
             1   1             ~ iwave, mbien
             1   3   4   3     ~ i,n,k,z
             2   5   6   1     ~ i,n,k,z
             3   1   2         ~ i,n,k
             1   1             ~ imbien, mrpeat

             3   2   1         ~ sample, mfilm, mwave
             1   1             ~ iwave, mbien
```

```
            1   3   4   4      ~ i,n,k,z
            2   5   6   1      ~ i,n,k,z
            3   1   2          ~ i,n,k
            1   1              ~ imbien, mrpeat

   5   1   1   1   1 ~ mangl, repeat,ambient,wave,sample/ (phi,delta,psi)
1     69.9970     0.0020    94.3800      0.0000     23.3700      0.0000
2     70.0000     0.0020    93.8200      0.0000     23.4300      0.0000
3     70.8500     0.0020    90.2900      0.0100     23.3400      0.0000
4     70.8500     0.0020    89.7700      0.0100     23.3900      0.0000
5     70.8900     0.0020    90.0600      0.0100     23.3400      0.0000
   3   1   1   1   2 ~ mangl, repeat,ambient,wave,sample/ (phi,delta,psi)
1     69.9970     0.0020    79.0900      0.0000     41.9600      0.0000
2     67.2000     0.0020    89.4400      0.0100     42.2400      0.0000
3     67.0300     0.0020    90.0900      0.0000     42.2800      0.0000
   2   1   1   1   3 ~ mangl, repeat,ambient,wave,sample/ (phi,delta,psi)
1     70.0000     0.0020    78.8580      0.0000     41.9780      0.0000
2     67.2000     0.0020    89.2900      0.0100     42.2500      0.0000

 zoom:   loop,    ratio of reduction,     |g|
                 (rel)       (total)
            0                           3.779E-01    (degrees)
            1   8.901E-01   8.901E-01   3.363E-01
            2   8.964E-01   7.979E-01   3.015E-01
            3   9.026E-01   7.202E-01   2.721E-01
            4   9.098E-01   6.552E-01   2.476E-01
            5   9.178E-01   6.013E-01   2.272E-01
            6   9.264E-01   5.570E-01   2.105E-01
            7   9.353E-01   5.210E-01   1.969E-01
            8   9.443E-01   4.920E-01   1.859E-01
            9   9.528E-01   4.688E-01   1.771E-01
           10   9.608E-01   4.504E-01   1.702E-01
           11   9.680E-01   4.360E-01   1.648E-01
           12   9.751E-01   4.251E-01   1.607E-01
           13   9.799E-01   4.166E-01   1.574E-01
           14   9.841E-01   4.100E-01   1.549E-01
           15   9.875E-01   4.048E-01   1.530E-01
           16   9.902E-01   4.009E-01   1.515E-01
           17   9.924E-01   3.978E-01   1.503E-01
           18   9.941E-01   3.955E-01   1.494E-01
           19   9.955E-01   3.937E-01   1.488E-01
           20   9.965E-01   3.923E-01   1.482E-01
           21   9.977E-01   3.914E-01   1.479E-01
           22   9.982E-01   3.907E-01   1.476E-01
           23   9.985E-01   3.901E-01   1.474E-01
           24   9.989E-01   3.897E-01   1.472E-01

 model parameter value along the minimum:
  1)         2.7520       0.07364   for:    5,  (n+ik), estimated uncertainty
  2)         1.3947       0.05952   for:    1,  (z    ), estimated uncertainty
  3)        50.3074       0.07289   for:    2,  (z    ), estimated uncertainty
  4)       100.3102       0.08841   for:    3,  (z    ), estimated uncertainty
```

```
 5)       100.2753      0.06702   for:    4,   (z    ), estimated uncertainty

initial |g| =   3.77889E-01    (degrees)
  final |g| =   1.47246E-01

------------------------------------------------------------
Statistics of deviations ~ experiment-model ~ g

   where:    g ~ column array of length ~ 2M
     let:   () ~ (psi or delta) ~ (1 or 2)

       mean () = m() = <g()> = (1/M) sum: g()
   variance () = < [g( )-m( )]**2 >
 covariance    = < [g(1)-m(1)]*[g(2)-m(2)] >
       std dev = sqrt (variance)
 correlat coef = covariance / [std dev (psi) * std dev (delta)]

                       mean,     std dev     (degrees)
      psi:            0.038        0.032
    delta:            0.016        0.202
                      0.553 ~ correlation coefficient ~ <psi|delta>

J(T)*J:          (renormalized for correlation)
   1)     1.00000
   2)    -0.98359   1.00000
   3)    -0.85950   0.87291   1.00000
   4)    -0.36403   0.27236   0.00000   1.00000
   5)    -0.29498   0.22193   0.00000   0.00000   1.00000

Normalization coefficients:      sqrt [J(T)*J](i,i)
  6.72E-03  8.21E-03  6.48E-03  4.09E-03  3.29E-03

rcond=   9.902E-05,  condition number

elapsed cpu-time = 64 centi-seconds
                 +  7 seconds
```

Some of the intermediate values contained in TEST.OUT may differ from the values above depending on the versions of VMS and FORTRAN that are used. Differences in calculated thicknesses and indices of refraction should be minimal.

MAESTRO also produces X.NAM and X.PRM files. On the lines after the first line, the X.NAM file contains the sample numbers or measurement descriptors which appear on alternate lines in the raw data file. These are used to label the table of data in the X.RES file. The first line of the X.NAM file contains a number equal to the number of parameters which are being varied in the MAIN1 calculation apart from the individual layer thicknesses.

```
$ TYPE TEST.NAM
   2
 TEST #1431
```

```
 TEST #1323  nist
 TEST #1323  test
```

The X.PRM file contains the model parameters as they appear in the opening lines of the X.DAT file.

```
$ TYPE TEST.PRM
   1
   1     632.800
   1
   1     1.00027
   6
   1    3.8750      0.0000    0
   2    0.0156      0.0000    0
   3    1.4620      0.0020    0
   4    0.0000      0.0000    0
   5    2.8000      0.0020    1
   6    0.0000      0.0000    0
```

The final results are given in the X.RES file. The first line of the X.RES file contains the file specifier of the X.RES file. Following that come the model parameter values and estimated uncertainties which are common or pooled over the entire set of measurements. In this case, model parameters 1 and 2 are the real part of the index of refraction and the thickness of the interlayer. Following them are the thickness measurements and uncertainties relating to the three groups of ellipsometric data, each group preceded by the pertinent measurement descriptor. The final |g| is a goodness of fit parameter discussed in section 3 of [1]. The significance of psi and delta is also discussed in section 3 of [1].

```
$ TYPE TEST.RES
 Results file is TEST.RES.

   1
   1     632.800
   1
   1     1.00027
   6
   1    3.8750      0.0000    0
   2    0.0156      0.0000    0
   3    1.4620      0.0020    0
   4    0.0000      0.0000    0
   5    2.8000      0.0020    1
   6    0.0000      0.0000    0

 model parameter value along the minimum:
   1)         2.7541      0.09684   for:    5,  (n+ik), estimated uncertainty
   2)         1.3502      0.08274   for:    1,  (z   ), estimated uncertainty
     TEST #1431
   3)        50.3172      0.02554   for:    2,  (z   ), estimated uncertainty
     TEST #1323  nist
```

```
   4)        100.3116      0.05889  for:    3,  (z    ), estimated uncertainty
     TEST #1323  test
   5)        100.2781      0.04649  for:    4,  (z    ), estimated uncertainty

   final |g| =  1.47414E-01

                        mean,      std dev      (degrees)
       psi:           0.039        0.031
     delta:           0.018        0.202
```

This completes this example run.

MAIN1 also produces the plot file X.PLOT (X.PLO in the MS-DOS version), however this file is not used by MAESTRO. See reference [1] for further information on this file. This completes this example run.

(In the VMS version, if files having the filename(s) specified on the MAESTRO command line already exist, new versions are created. In the MS-DOS version, however, if a file having a .DAT, .NAM, .PRM, .OUT, .PLO, or .RES extension already exists, that file is renamed to a file having a .DAX, .NAX, .PRX, .OUX, .PLX, or .REX extension, respectively. MAESTRO prints a message to indicate that the renaming is occurring. This gives the user one chance to recover from a situation in which files would otherwise be overwritten.)

6. INPUTTING DATA FILE SPECIFIERS INDIVIDUALLY

Let us run another example to show how the file specifiers containing the ellipsometric data can be entered interactively.

$ MAESTRO TEST P

So that the X.DAT file will be the same as the one already created, we use the PARAMS.MOD file which we also created above.

```
Enter the file specifier of the file containing the model parameters.
PARAMS.MOD

Type 0 to EXIT
     1 to generate X.DAT from the current model parameters
     2 to view the current model parameters
     3 to modify the current model parameters
1
```

Selecting option 1 above allows us to proceed directly to the generation of the X.DAT file.

```
Type 1 to enter the file specifiers and nominal
       oxide thicknesses interactively, or
     2 to enter the file specifer of a file
       containing this information.
1
```

This time we will name file data files individually. We first tell MAESTRO how many data files there are. Then we name them and enter the nominal thickness of the oxide layer that goes with each file.

```
How many data files contain the data?
2
Enter the file descriptor of file #  1
TEST50.DAT

Enter the nominal oxide thickness in nm of
  the wafers whose data are in file #  1
50

Enter the file descriptor of file #  2
TEST100.DAT

Enter the nominal oxide thickness in nm of
  the wafers whose data are in file #  2
100
```

Since we have entered all the file specifiers and thicknesses, MAESTRO allows us to write this information to a file so that we will not have to enter it the next time we run MAESTRO.

```
Do you want to write the list of data file specifiers
  and thicknesses to a file which MAESTRO will be able
  to read directly?  Answer Y or N.
Y

Enter file specifier.
TEST.FIL
FORTRAN STOP

File TEST.DAT has been prepared successfully.
```

(In the MS-DOS version, if a file by that name already exists, a message appears asking the user whether or not MAESTRO should overwrite that existing file. The user may answer 'Y' to overwrite or 'N' to be prompted for another file descriptor.)

This completes this run of MAESTRO. Below is the TEST.FIL file which was created and which can be used the next time we run MAESTRO. The TEST.FLS (see section 4.6) and TEST.FIL files are identical in function. The thickness values are placed farther right in the records of TEST.FIL to permit long VMS file specifiers.

```
$ TYPE TEST.FIL
TEST50.DAT                                          50.0000
TEST100.DAT                                        100.0000
```

7. THE CASE OF NO INTERLAYER

A third example will be used to illustrate another feature. If the thickness, uncertainty, and 'vary flag' of the interlayer are all set to 0, MAESTRO assumes that there is no interlayer, and the X.DAT file is built to represent a single layer on a substrate.

```
$ MAESTRO TEST P

Enter the file specifier of the file containing the model parameters.
PARAMS.FIL

Type 0 to EXIT
     1 to generate X.DAT from the current model parameters
     2 to view the current model parameters
     3 to modify the current model parameters
3

Type in new values in response to the following
  prompts.  Press RETURN to keep old values.

Wavelength, nm = 632.800                        >
n of air = 1.00027                              >
n of silicon = 3.8750                           >
Unc. of n of silicon = 0.0000                   >
Vary flag for n of silicon = 0                  >
k of silicon = 0.0156                           >
Unc. of k of silicon = 0.0000                   >
Vary flag for k of silicon = 0                  >
n of SiO2 = 1.4620                              >
Unc. of n of SiO2 = 0.0020                      >
Vary flag for n of SiO2 = 1                     >
k of SiO2 = 0.0000                              >
Unc. of k of SiO2 = 0.0000                      >
Vary flag for k of silicon = 0                  >
n of interlayer = 2.8000                        >
Unc. of n of interlayer = 0.0020                >
Vary flag for n of interlayer = 1               >
k of interlayer = 0.0000                        >
Unc. of k of interlayer = 0.0000                >
Vary flag for k of interlayer = 0               >
Thickness of interlayer, nm = 1.0000            > 0
Thickness of interlayer changed from 1.0000 to 0.0000

Unc. of thickness of interlayer = 0.5000        > 0
Unc. of interlayer thickness changed from 0.5000 to 0.0000

Vary flag for thickness of interlayer = 1       > 0
Vary flag for interlayer thickness changed from 1 to 0
```

The thickness, uncertainty of the thickness, and thickness 'vary flag' for the interlayer have all been set to zero.

```
Type 0 to EXIT
     1 to generate X.DAT from the current model parameters
     2 to view the current model parameters
     3 to modify the current model parameters
     4 to write altered model parameters to a new file
1

Type 1 to enter the file specifiers and nominal
       oxide thicknesses interactively, or
     2 to enter the file specifier of a file
       containing this information.
2
Enter file specifier of file containing data
  file specifiers and nominal thicknesses.
TEST.FIL
```

Note that we are using the TEST.FIL file which was generated by MAESTRO in an earlier example.

```
FORTRAN STOP

File TEST.DAT has been prepared successfully.
```

8. ERROR MESSAGES

The three component programs of MAESTRO each have error messages associated with them. These messages are combined in the following listing and are shown in bold followed by an explanation. In some cases, the error message may occupy more than one line even though printed on a single line below.

Answer Y, y, N, or n. These are the only responses allowed to this prompt.

Cannot find file <file>. The model parameter file, ellipsometric data file, or file of data file specifiers could not be found.

The character <char> is not allowed -- Exiting. Only the characters P, p, X, and x can appear in the last parameter of the MAESTRO command. (This message does not appear in the MS-DOS version.)

The command must have either two or three parameters following it. The MAESTRO command must be followed by either one or two filenames and a type_mode string (P, X, PX, or XP).

Each of the letters P and X can appear only once. More than one P or X appears in the last parameter of the MAESTRO command. (This message does not appear in the MS-DOS version.)

File specifier in record <number> is > 50 characters. The file containing data file specifiers contains a file specifier which is more than the maximum permitted 50 characters.

Illegal entry. The response to the prompt must be an integer in the range 0 to 3 or 0 to 4 depending on circumstances.

MAESTRO aborted. Indicates that MAESTRO execution has stopped. This message usually follows another error message or results from a control-Y interrupt.

MAESTRO (or MAESDOS) did not complete normally. The MAESTRO.EXE (or MAESDOS.EXE) executable did not run to normal completion.

Number entered must be 1 or 2. The response to the prompt must be either a 1 or a 2.

The number of data files cannot be less than 1 or greater than 50. There must be at least one but no more than 50 files containing ellipsometric data.

Odd number of records encountered in file <file>. The ellipsometric data file must be organized in pairs with measurement descriptor record followed by data record.

Parameter file ends before 23 values are read. The parameter file contains fewer than 23 parameter values, that is, fewer than 23 uncommented lines.

Record <number> contains no thickness value. A record in the file of file specifiers contains no thickness value following the file specifier.

Record <number> truncated at 80 characters. A record in the file of file specifiers contains a non-space character in character position 80. Any characters beyond that are truncated.

String containing "final |g|" not found. MAIN1 did not produce the expected X.OUT file. This message is written to the .RES file.

String containing "model parameter . . ." not found in X.OUT file. MAIN1 did not complete normally. STOF could not find the indicated string in the X.OUT file. This probably means that MAIN1 did not complete normally. This message is written to the .RES file.

String containing "mean, std dev" not found. MAIN1 did not produce the string "mean, . . . std dev" in the X.OUT file. This message is written to the .RES file.

(**<String> is not a legal type_mode. Must be P, X, PX, or XP in all upper** or **all lower case.** The final argument of the MAESTRO command must be some combination of X and P with no mixed cases permitted on PX or XP.)

<String>.DAT was not found. The file having the filename given by the first parameter in the MAESTRO command could not be found.

There are more than 150 sets of ellipsometric data. As configured, MAESTRO and MAIN1 are limited to 150 sets of ellipsometric data.

There are more than 50 file specifiers. The program cannot process data from more than 50 files.

The X.NAM file could not be found. It must be in your current directory. The STOF program could not find the X.NAM file. Perhaps your default directory is not properly set. This message is written to the .RES file.

The X.OUT file could not be found. It must be in your current directory. The STOF program could not find the X.OUT file. Perhaps your default directory is not properly set. This message is written to the .RES file.

Unable to create JOBFILE, possibly due to directory protection. This message could appear if you do not have write access to the default directory. (This message does not appear in the MS-DOS version.)

9. LIMITATIONS

Additional information on MAESTRO is contained in the opening comments to the MAESTRO.FOR and MAESDOS.FOR programs. Part of this covers some of the limitations of the program and is reproduced below. Some of these also appear elsewhere in the text.

> Psi and Delta data on each wafer are considered independently as they pertain to calculating the oxide layer thickness for that particular wafer, even though measurements may be made at multiple angles.
>
> Data for a given wafer are identified by having the same sample number or measurement descriptor. A change in measurement descriptor signifies that a new set of multiple-angle measurements is about to begin.
>
> Each individual data file contains data from wafers having a common nominal oxide thickness, although multiple data files can be accommodated in a single MAIN1 run. The maximum number of data files permitted is 50.
>
> Among the 50 (or fewer) data files, there can be no more than 150 sets of ellipsometric data.
>
> The file specifier of the data files and the parameter file cannot be more than 50 characters long. In the file of file specifiers, each file specifier must begin in column 1.
>
> The sample number information in the ellipsometric data file is assumed to not go beyond character position 30.
>
> The ellipsometer readings in the data file are assumed to not go beyond character position 75.
>
> MAIN1 runs in mode 2, an unconstrained optimization.
>
> The uncertainty in the layer thickness model parameters is 0.5 nm.

Data for a particular sample are all contained in a single file and do not carry over into a succeeding file.

10. INSTALLATION

The VMS version of MAESTRO is available on half-inch tape at 800 bpi or 1600 bpi density. The tape includes FORTRAN sources, executables, the MAESTRO.COM file, and the files created in the example of sections 4 and 5. Installation is as follows:

```
$ ! Create a directory to contain all the files.  In this
$ ! example, it is called [DIR2].
$ SET DEFAULT [DIR2]
$ ALLOCATE MTA0:        ! or other tape drive
$ MOUNT/FOR/NOWRITE MTA0:
$ BACKUP/VER/REWIND MTA0:MAESTRO.BCK []
$ FORTRAN MAESTRO       ! Compile and link are optional.  You may
$ FORTRAN FSREAD        ! use the supplied MAESTRO.EXE file.
$ FORTRAN PARSUB
$ FORTRAN MPARM
$ FORTRAN RPARM
$ FORTRAN VPARM
$ FORTRAN WPARM
$ LINK MAESTRO,FSREAD,PARSUB,MPARM,RPARM,VPARM,WPARM
$ DISMOUNT MTA0:
$ DEALLOCATE MTA0:
$ ! End of installation.
```

You must now edit the MAESTRO.COM file, set the default directory, and define the MAESTRO symbol as explained in section 4.1.

The files for the VMS version are also available on personal computer diskette. The user may transfer them to the VAX using Kermit or some other file transfer protocol.

(The files for the MS-DOS version are available on 3.5-inch 1.44-MB personal computer diskette. All program and example files are on the diskette. MAESTRO can be run from the supplied diskette provided the Salford run-time library is loaded as explained earlier. The files may be copied to a convenient directory on a hard disk. The files MAESDOS.EXE, STOF2.EXE, and MAESTRO.BAT must be in the path. Should it be necessary to recompile MAESDOS, use the COMPILE.BAT procedure. To relink, type LINK77 MAESDOS.LNK at the DOS prompt.)

11. ACKNOWLEDGMENTS

The author is indebted to Jay F. Marchiando for valuable discussions regarding the operation of MAIN1, and to Barbara J. Belzer for a thorough critique of this document which included various test runs of the program with outputs carefully examined.

12. REFERENCES

[1] Marchiando, J. F., Semiconductor Measurement Technology: A Software Program for Aiding the Analysis of Ellipsometric Measurements, Simple Models, NIST Special Publication 400-83, July 1989.

NIST-114A
(REV. 3-90)

U.S. DEPARTMENT OF COMMERCE
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY

BIBLIOGRAPHIC DATA SHEET

1. PUBLICATION OR REPORT NUMBER
NISTIR 4969

2. PERFORMING ORGANIZATION REPORT NUMBER

3. PUBLICATION DATE
December 1992

4. TITLE AND SUBTITLE
MAESTRO: A Front-End to the MAIN1 Program for Multiple-Angle Measurement of Silicon Dioxide Layers

5. AUTHOR(S)
R. L. Mattis

6. PERFORMING ORGANIZATION (IF JOINT OR OTHER THAN NIST, SEE INSTRUCTIONS)
U.S. DEPARTMENT OF COMMERCE
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
GAITHERSBURG, MD 20899

7. CONTRACT/GRANT NUMBER

8. TYPE OF REPORT AND PERIOD COVERED

9. SPONSORING ORGANIZATION NAME AND COMPLETE ADDRESS (STREET, CITY, STATE, ZIP)

10. SUPPLEMENTARY NOTES

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.)

MAESTRO is an interactive program which serves as a front-end to the MAIN1 computer program for processing ellipsometric data. It is applicable when MAIN1 is used to characterize silicon dioxide layers on silicon substrates using a single pair of Delta-psi values, using repeated pairs of Delta-psi values taken at the same nominal angle of incidence, or using pairs of Delta-psi values taken at multiple angles of incidence. MAESTRO stands for Multiple-Angle Ellipsometry for Supplying Thickness and Refractive index Output. It consists of two FORTRAN programs and a VMS DCL command procedure. An implementation for MS-DOS is also available. MAESTRO is used to prepare the X.DAT file required by MAIN1 and to give this file and the MAIN1 output files user-defined names.

12. KEY WORDS (6 TO 12 ENTRIES; ALPHABETICAL ORDER; CAPITALIZE ONLY PROPER NAMES; AND SEPARATE KEY WORDS BY SEMICOLONS)
ellipsometry; FORTRAN; index of refraction; layer thickness; modeling; standards

13. AVAILABILITY

- [x] UNLIMITED
- [ ] FOR OFFICIAL DISTRIBUTION. DO NOT RELEASE TO NATIONAL TECHNICAL INFORMATION SERVICE (NTIS).
- [ ] ORDER FROM SUPERINTENDENT OF DOCUMENTS, U.S. GOVERNMENT PRINTING OFFICE, WASHINGTON, DC 20402.
- [x] ORDER FROM NATIONAL TECHNICAL INFORMATION SERVICE (NTIS), SPRINGFIELD, VA 22161.

14. NUMBER OF PRINTED PAGES
25

15. PRICE
A02

ELECTRONIC FORM