ALS Data Analysis
Revision 1.1

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Contents

1 Introduction

These notes give instructions about how to analyze the data from ALS. Some parts would probably also be applicable to analyzing data from the BYU reflectometer. The notes take you through the process of copying the data from ALS (Section 2), converting the raw data to reflectance (Section 3), and fitting the data (Section 4).

I am assuming that you already have an account on volta and that you will be using volta for your acquisition and analysis. If you need a volta account, please see me. I will either create a personal one for you or give you the username and password for the group account. I have included a brief unix and x-windows survival guide in Section 5) in case you need a reminder about living inside of unix.

2 Copying Data

This section describes how to transfer data to and from the ALS data acquisition computer in Beamline 6.3.2 to a Windows PC (Section 2.1) or to volta (Section 2.2). Please be careful with the login names and passwords needed for this transfer. The data acquisition programs at ALS could be compromised if someone malicious gets access to them.

2.1 PC Transfer

You can establish a connection between a PC in N212 ESC and the computer at ALS much the same way you would connect to volta. It is a little simpler because we are only worried about file transfer and need not bother with the x-windows stuff.

1. Start the secure file transfer client. This is probably on the Desktop as an icon. If it is not, click on
   Start/All Programs/SSH Secure Shell/Secure File Transfer Client.

2. Click on the Quick Connect menu item at the top of the window.

3. Fill in the dialog box with the host name of `metro1.als.lbl.gov` the user name you can get from me. The character after 'metro' is the digit '1' than than the letter 'l'.

4. You will probably get a warning message about the computer using an insecure version of secure shell. If so, click `OK` to accept that connection.

5. A secure shell client window will pop and asking your for a password in a dialog box. You can get the password from me. The case matters in the password.

You can use the secure shell client to transfer files back and forth between the PC you are working on and metro1. The left-hand pane will list files on the PC you can upload to volta by right-clicking on the file and selecting "upload dialog." The right-hand pane will list files on volta you can download to the PC by right-clicking on the file and selecting the "download dialog."

2.2 Volta Transfer

Transfers between volta and metro1 are accomplished with the unix `ftp` command (file transfer protocol). I have listed a log of an ftp session below with an explanation following.

```
volta.byu.edu> ftp metro1.als.lbl.gov
Connected to metro1.als.lbl.gov (131.243.72.103).
220 metro1.als FTP server (SunOS 5.6) ready.
Name (metro1.als.lbl.gov:turley): XXXXX (get username from me)
331 Password required for XXXXXX.
Password: (will not echo)
230 User XXXXXXX logged in.
Remote system type is UNIX.
Using binary mode to transfer files.
ftp> cd Shannon/uox03
250 CWD command successful.
ftp> get uox03.log
local: uox03.log remote: uox03.log
227 Entering Passive Mode (131,243,72,103,183,106)
150 Binary data connection for uox03.log (128.187.201.121,40651) (35139 bytes).
226 Binary Transfer complete.
35139 bytes received in 0.282 secs (1.2e+02 Kbytes/sec)
ftp> prompt
Interactive mode off.
ftp> mget *.dat
.
.
.
226 Binary Transfer complete.
933 bytes received in 0.00279 secs (3.3e+02 Kbytes/sec)
local: uox03000131.dat remote: uox03000131.dat
227 Entering Passive Mode (131,243,72,103,183,238)
150 Binary data connection for uox03000131.dat (128.187.201.121,40784) (1360 bytes).
226 Binary Transfer complete.
1360 bytes received in 0.00335 secs (4e+02 Kbytes/sec)
ftp> quit
221 Goodbye.
volta.byu.edu>
```

The `ftp` command establishes a file transfer connection between the ALS computer metro1 and volta. Make sure to distinguish between the digit '1' in 'metro1' and the letter 'l' in 'lbl'. The password will not echo on the screen. Be sure to safeguard the password since an unauthorized person could use it to cause trouble on the data acquisition computer at ALS. The first ftp command is the same as the unix `cd` command. It changes the default directory to `Shannon/uox03`. `Shannon` is the current user name for our group on the computer and the name of the directory with all of our projects. The subdirectory `uox03` contains the data for the data project on 3/15/03. The `get` command copies the file `uox03.log` to the current directory on volta. It has a lot of useful information about each of the data runs. The `prompt` command turns off verification from the user during wildcard copies. Without it, ftp would ask you on each file if you were sure you wanted to transfer it. The `mget` command is like get, but it allows wildcards. It copies all of the data files from the `uox03` project to the current directory. The `quit` command exits the `ftp` program and returns to the volta command prompt. You can read about other ftp command and options by typing `man ftp`.

3 Reflectance Calculations

Once you have the data files from LBL, you need to generate a data file with the reflectance information. Matt McDonald wrote a FORTRAN program that will do this for us. I have modified the program to add graphics and improve the dark current subtraction in a way that allows the dark current to vary with angle. Instructions on how to run the program are in Section 3.1.

You may be okay generating a reflectance file using Excel on the PC if you prefer. I include some brief instructions in Section 3.2) about the algorithms (without detailed Excel instructions) if you would like to do this on your own.

3.1 Running the reflect Program

The `reflect` program converts raw ALS data into reflection data files that can be used in the `alsfit` fitting program (see Section 4). It is located in the unix directory `/usr/local/bin` so it should already be in your path. It will first ask you for the wavelength. Respond with the wavelength of the data in Angstroms. It next prompts for the root file name. This is the project name (if the files are in your current working directory) or the absolute path plus the project name (if the data files are in another directory). It then asks for the ALS run number. This is the run number for the unnormalized sample reflectance. It then asks if you want to do a dark current correction (recommended). Supply it with the slope and intercept of the dark current data. This assumes you have already fit this with Excel or another program. Next it asks for the run number for the ALS normalization data (I0). Finally, it asks for the output file. This is a name you invent that will be used as the input for the fitting program.

3.2 Reflection Algorithms

The reflectance of the samples if given by

$$R = \frac{(z_i - z_d(\theta)) * I_0}{(z_0 - z_d(\theta)) * I_i} \, , \tag{1}$$

where

- z_i is the diode current in the reflected beam
- $z_d(\theta)$ is the angle-dependent dark current
- I_0 is the beam current from the normalization run
- z_0 is the diode current from the normalization run
- I_i is the beam current from the reflected beam run

Nick, Luke, and I have found that a linear fit to the dark current using a run with the same gain as the reflected beam run (and the same energy, filter, etc.) gives the best results.

4 Fitting Data

The data can be fit by running the `alsfit` program. It assumes that you already have converted the raw ALS data to a reflectance data file (see Section 3.1). It can do a least-squares fit and error estimation on your data using the minuit library. I will give a description here about one way to run the program and some of the basic minuit commands. I recommend reading the miniut instruction manual to get more detailed instructions.

Start the program by typing `minuit` from the directory where you want to analyze your data. It is probably convenient to have it be the same directory as the input data files.

4.1 Parameter Input

The program will then prompt you to enter a minuit title or "SET INPUT n". You can save yourself a lot of time by setting up an input parameter file that gives you a good start on the fit parameters. I will give examples of both ways to enter parameter data below for a sample that has a V film with a VO layer on top.

4.1.1 Manual parameter input

For manual parameter input (the slow way) respond to the

```
ENTER MINUIT TITLE, or "SET INPUT n" :
```

with a title of your choice to identify the data.

```
Example run
 Example run
 ********************************************************************************
 ENTER MINUIT PARAMETER DEFINITION:
```

You now need to enter each of the fit parameters you will be using. The program listed how these are numbered when it first started up:

```
For this version of the program, the input parameters
as follows:
1: estimated sigma^2 for fit
2: thickness of SiO2 layer
3: n for first film
4: k for first film
5: thickness of first film
6...: repeat for additional films
```

There are a couple of different kinds of parameters the program can use. For this example, we will use constants, unconstrained fit parameters, and constrained fit parameters.

Parameter 1 is σ^2 for the fit. Eventually it should be adjusted so the χ^2 is equal to the number of data points minus the number of fit parameters. The program prints out the current value of χ^2 is `FCN` (if you are interested, Section 4.5 lists the formulas used to calculate FCN). A good starting value for parameter 1 is a constant value of 1. This is specified by typing

```
1 'sigma^2' 1
```

The program will respond with

```
     1 'sigma^2   '    1.0000      constant
 ENTER MINUIT PARAMETER DEFINITION:
```

The next parameter is the thickness of the SiO_2 layer, which we will set to the constant value of 18 Å.

```
2 'tSiO2' 18
     2 'tSiO2     '    18.000      constant
 ENTER MINUIT PARAMETER DEFINITION:
```

The label in quotes can be whatever you want to use to describe what this fit parameter is. The next parameter is the index real part of the index of refraction of the V film. I will try a starting value of 0.9 which I think is likely accurate to about 0.1. I will not constrain the value of the parameter in the fit.

```
3 'nV' 0.9 .1
     3 'nV        '   0.90000      0.10000         no limits
 ENTER MINUIT PARAMETER DEFINITION:
```

The imaginary part of the V index of refraction is probably within about 0.05 of 0.1. I have physical doubts about the possibility of it being less than 0 or greater than 0.5. I will specify it as a fit parameter with those constraints.

```
4 'kV' 0.1 .05 0 .5
     4 'kV        '   0.10000      0.50000E-01     0.0000      0.50000
 ENTER MINUIT PARAMETER DEFINITION:
```

Filling in the rest of the parameters I have

```
 ENTER MINUIT PARAMETER DEFINITION:
5 'tV' 150 30
     5 'tV        '    150.00       30.000         no limits
 ENTER MINUIT PARAMETER DEFINITION:
6 'nVO' 0.9 .1
     6 'nVO       '   0.90000      0.10000         no limits
 ENTER MINUIT PARAMETER DEFINITION:
7 'kVO' 0.1 .05 0 .5
     7 'kVO       '   0.10000      0.50000E-01     0.0000      0.50000
 ENTER MINUIT PARAMETER DEFINITION:
8 'tVO' 50 20
     8 'tVO       '    50.000       20.000         no limits
 ENTER MINUIT PARAMETER DEFINITION:
```

This completes the sets of parameters I want to initialize. I can move on to the next phase of the program by responding with a blank line to the prompt. The program will then ask me for information about the data I will be fitting. I have a data file named `101.txt` which contains data taken at a wavelength of 100 Å.

```
 MINUIT: FIRST CALL TO USER FUNCTION, WITH IFLAG=1
input file name: 101.txt
          72  data points read in
wavelength: 100 Mirror structure: Enter 0 for a single layer, n>0
for a multilayer with n layer pairs, or -1 for the end of the
stack. Layers are ordered from the substrate to the surface.
element  1:
```

The program now wants to know the structure of my mirror. I have two films, V and VO. If I had multilayers, I could respond to the prompt with the number of layer-pairs in each multilayer instead of with 0 as I do below.

```
element  1: 0 element  2: 0 element  3: -1

 FCN=  0.6494880E-02 FROM PARAMETR  STATUS=RESET          2 CALLS        2 TOTAL
                     EDM= unknown      STRATEGY= 1      NO ERROR MATRIX
```

```
  EXT PARAMETER                CURRENT GUESS      PHYSICAL LIMITS
  NO.   NAME        VALUE          ERROR       NEGATIVE      POSITIVE
   1    tSiO2       18.000       constant
   2    tSiO2       18.000       constant
   3    nV         0.90000       0.10000
   4    kV         0.10000       0.50000E-01    0.0000       0.50000
   5    tV          150.00        30.000
   6    nVO        0.90000       0.10000
   7    kVO        0.10000       0.50000E-01    0.0000       0.50000
   8    tVO         50.000        20.000
 ENTER MINUIT COMMAND:
```

I am now ready to fit my data.

4.1.2 Parameter file input

I can save myself the tedium of typing in all of the above commands every time I run the program. I have created a file called `als.in` which has the following contents.

```
set title
Example run
param
1 'sigma2' 1
2 'tSiO2' 18
3 'nV' .9 .1
4 'kV' .1 .05 0 .5
5 'tV' 150 30
6 'nVO' .9 .1
7 'kVO' .1 .05 0 .5
8 'tVO' 50 20
```

By responding to the first `minuit` prompt with a set input response, I can use the data in this file as follows

```
 ENTER MINUIT TITLE, or "SET INPUT n" :
set input 3
 **********
 **    1 **set input 3
 **********
 UNIT NO. :3
 UNIT  3 IS NOT OPENED.
 NO FILE NAME GIVEN IN COMMAND.
 PLEASE GIVE FILE NAME:
als.in
```

```
 FILE OPENED SUCCESSFULLY.
 SHOULD UNIT  3 BE REWOUND?
n
 Example run
 ********************************************************************************

 PARAMETER DEFINITIONS:
    NO.   NAME         VALUE      STEP SIZE      LIMITS
     1 'sigma2    '    1.0000      constant
     2 'tSiO2     '    18.000      constant
     3 'nV        '   0.90000      0.10000          no limits
     4 'kV        '   0.10000      0.50000E-01      0.0000      0.50000
     5 'tV        '    150.00       30.000          no limits
     6 'kVO       '   0.90000      0.10000          no limits
     7 'nVO       '   0.10000      0.50000E-01      0.0000      0.50000
     8 'tVO       '    50.000       20.000          no limits
    ********************************************************************************

 MINUIT: FIRST CALL TO USER FUNCTION, WITH IFLAG=1
input file name:
```

I then proceed from this point as noted in the previous section.

If you would like to change a few of the parameters from their default values, you can do so after you finish with the section for reading in the data. To do this you use the `set par` command. For instance, let's say I wanted to change the initial value of parameter 3 to 0.91.

```
 END OF DATA ON UNIT NO.  3
 INPUT WILL NOW BE READ IN INTERACTIVE MODE FROM UNIT NO.  5
 FILENAME: unknown
 ENTER MINUIT COMMAND:
set par 3 0.91
 **********
 **    2 **SET PAR    3.000      0.9100
 **********
 ENTER MINUIT COMMAND:
```

I can verify this change took place with the `show par` command.

```
 show par
 **********
 **    3 **SHOW PAR
 **********

 FIRST CALL TO USER FUNCTION AT NEW START POINT, WITH IFLAG=4.
```

```
 FCN=  0.1257118     FROM SET PARM  STATUS=NEW VALUES     1 CALLS        3 TOTAL
                     EDM= unknown      STRATEGY= 1      NO ERROR MATRIX

  EXT PARAMETER               CURRENT GUESS      PHYSICAL LIMITS
  NO.   NAME        VALUE          ERROR       NEGATIVE      POSITIVE
   1    sigma2      1.0000       constant
   2    tSiO2       18.000       constant
   3    nV         0.91000       0.10000
   4    kV         0.10000       0.50000E-01    0.0000       0.50000
   5    tV          150.00        30.000
   6    kVO        0.90000       0.10000
   7    nVO        0.10000       0.50000E-01    0.0000       0.50000
   8    tVO         50.000        20.000
 ENTER MINUIT COMMAND:
```

To change the uncertainty on parameter 3, I have to use the `par` command.

```
par
 ENTER MINUIT PARAMETER DEFINITION:
3 'nV' 0.91 .05
     3 'nV        '   0.91000      0.50000E-01     no limits
 ENTER MINUIT PARAMETER DEFINITION:

 ENTER MINUIT COMMAND:
```

I am now ready to start fitting the data.

4.2 Fitting

After the data is read in and the parameters are set, you can begin fitting the data. Usually you will do this with the `migrad` command. If this doesn't work, there are a couple of other commands that may narrow in your choices such as `simplex` or `simplex`. Consult the minuit manual for how these are used.

```
migrad
 **********
 **    5 **MIGRAD
 **********

 FIRST CALL TO USER FUNCTION AT NEW START POINT, WITH IFLAG=4.
 START MIGRAD MINIMIZATION.  STRATEGY 1.  CONVERGENCE WHEN EDM .LT. 0.10E-03

 FCN=  0.7734654E-01 FROM MIGRAD    STATUS=INITIATE     113 CALLS      117 TOTAL
                     EDM= unknown      STRATEGY= 1      NO ERROR MATRIX
```

```
 EXT PARAMETER                CURRENT GUESS       STEP         FIRST
 NO.   NAME        VALUE          ERROR          SIZE      DERIVATIVE
  1    sigma2      1.0000       constant
  2    tSiO2       18.000       constant
  3    nV          2.8733       0.50000E-01    0.0000       0.19023
  4    kV         0.16780E-03   0.50000E-01  -0.89065       0.34670E-02
  5    tV          150.00        30.000        0.0000       0.32487E-02
  6    kVO        0.90000       0.10000        0.0000       -2.3933
  7    nVO        0.10000       0.50000E-01    0.0000       0.43717
  8    tVO         114.89        20.000        0.0000       0.18115E-02

MIGRAD MINIMIZATION HAS CONVERGED.

MIGRAD WILL VERIFY CONVERGENCE AND ERROR MATRIX.
COVARIANCE MATRIX CALCULATED SUCCESSFULLY

FCN=  0.9734934E-02 FROM MIGRAD    STATUS=CONVERGED    322 CALLS      326 TOTAL
                    EDM=  0.70E-05    STRATEGY= 1      ERROR MATRIX ACCURATE

 EXT PARAMETER                                        STEP         FIRST
 NO.   NAME        VALUE          ERROR              SIZE      DERIVATIVE
  1    sigma2      1.0000       constant
  2    tSiO2       18.000       constant
  3    nV          2.8735        1.0645        0.91799E-04   0.87458E-02
  4    kV         0.16938E-05   0.30212        0.24033E-02   0.25884E-03
  5    tV          150.01        63.742        0.54735E-02   0.14422E-03
  6    kVO        0.92061       0.15467        0.16233E-04   0.99844E-01
  7    nVO        0.60013E-01   0.27319        0.15064E-03   0.96338E-02
  8    tVO         102.81        159.48        0.30372E-01   0.40811E-04

EXTERNAL ERROR MATRIX.    NDIM=  50    NPAR=  6    ERR DEF=  1.00
 0.113E+01 0.249E-04-0.658E+02-0.153E-02-0.130E-02-0.522E-01
 0.249E-04 0.241E-04 0.125E-02-0.894E-05-0.545E-05 0.782E-02
-0.658E+02 0.125E-02 0.406E+04-0.571E-01 0.466E-01-0.513E+03
-0.153E-02-0.894E-05-0.571E-01 0.239E-01-0.229E-01-0.180E+02
-0.130E-02-0.545E-05 0.466E-01-0.229E-01 0.285E-01 0.114E+02
-0.522E-01 0.782E-02-0.513E+03-0.180E+02 0.114E+02 0.254E+05

PARAMETER  CORRELATION COEFFICIENTS
      NO.  GLOBAL     3     4     5     6     7     8
       3  0.98139  1.000 0.005-0.969-0.009-0.007 0.000
       4  0.04957  0.005 1.000 0.004-0.012-0.007 0.010
       5  0.98156 -0.969 0.004 1.000-0.006 0.004-0.050
       6  0.97675 -0.009-0.012-0.006 1.000-0.877-0.730
       7  0.95437 -0.007-0.007 0.004-0.877 1.000 0.422
```

```
       8  0.91665  0.000 0.010-0.050-0.730 0.422 1.000
 ENTER MINUIT COMMAND:
```

This command accomplished a lot while we weren't looking!

4.3 Error Estimation

Once it found our minimum, it printed out the value of $\chi^2 = 0.973493 \times 10^{-2}$ and computed an approximate error matrix and correlation coefficients. Neither of these mean much yet, since our value of χ^2 is so far from the expected value. We would like to force it to be about equal to the number of data points minus the number of degrees of freedom. The value of FCN is divided by σ^2, so we will set that to .000012.

```
 ENTER MINUIT COMMAND:
set par 1 .000012
 **********
 **    3 **SET PAR    1.000      0.1200E-04
 **********
 ENTER MINUIT COMMAND:
migrad
 **********
 **    4 **MIGRAD
 **********

 FIRST CALL TO USER FUNCTION AT NEW START POINT, WITH IFLAG=4.
 START MIGRAD MINIMIZATION.  STRATEGY 1.  CONVERGENCE WHEN EDM .LT. 0.10E-03

 FCN=   260.3435     FROM MIGRAD    STATUS=INITIATE      30 CALLS      279 TOTAL
                     EDM=  0.18E+06  STRATEGY=1  ERROR MATRIX UNCERTAINTY=100.0%

  EXT PARAMETER                APPROXIMATE        STEP         FIRST
  NO.   NAME        VALUE          ERROR          SIZE      DERIVATIVE
   1    sigma2     0.12000E-04   constant
   2    tSiO2       18.000       constant
   3    nV         0.90371       0.33665       0.18621E-02    1651.3
   4    kV         0.37860E-01   0.27322       0.10072E-01    107.56
   5    tV          445.38        1266.3      -0.76744E-02   0.34657E-01
   6    kVO        0.91901       0.11887       0.62793E-03   -7815.0
   7    nVO        0.64064E-01   0.78486E-01  -0.11739E-02   -65.280
   8    tVO         21.767        332.74       -1.9860      -0.40602
 MIGRAD FAILS TO FIND IMPROVEMENT
 MINUIT WARNING IN HESSE
 ============== Negative diagonal element  3 in Error Matrix
 MINUIT WARNING IN HESSE
 ==============     0.10E+01 added to diagonal of error matrix
```

```
COVARIANCE MATRIX CALCULATED SUCCESSFULLY

FCN=   260.3435     FROM HESSE     STATUS=OK            40 CALLS      320 TOTAL
                    EDM=  0.76E+03    STRATEGY= 1      ERROR MATRIX ACCURATE

 EXT PARAMETER                                        STEP         FIRST
 NO.   NAME        VALUE          ERROR              SIZE      DERIVATIVE
  1    sigma2     0.12000E-04   constant
  2    tSiO2       18.000       constant
  3    nV         0.90371       0.14516E-02   0.33482E-04    1651.3
  4    kV         0.37860E-01   0.29915E-02   0.58062E-03    107.59
  5    tV          445.38        1.4144       0.20656       0.34657E-01
  6    kVO        0.91901       0.74592E-02   0.27321E-04   -7815.0
  7    nVO        0.64064E-01   0.11350E-01   0.16171E-04   -65.279
  8    tVO         21.767        4.3956       0.26233E-02  -0.40600

MIGRAD MINIMIZATION HAS CONVERGED.

MIGRAD WILL VERIFY CONVERGENCE AND ERROR MATRIX.
MINUIT WARNING IN HESSE
============== Negative diagonal element  3 in Error Matrix
MINUIT WARNING IN HESSE
==============     0.10E+01 added to diagonal of error matrix
COVARIANCE MATRIX CALCULATED SUCCESSFULLY

FCN=   64.48379     FROM MIGRAD    STATUS=CONVERGED    774 CALLS     1023 TOTAL
                    EDM=  0.39E-05    STRATEGY= 1      ERROR MATRIX ACCURATE

 EXT PARAMETER                                        STEP         FIRST
 NO.   NAME        VALUE          ERROR              SIZE      DERIVATIVE
  1    sigma2     0.12000E-04   constant
  2    tSiO2       18.000       constant
  3    nV         0.89796       0.28725E-02   0.28136E-05    2.9998
  4    kV         0.83976E-01   0.50808E-02   0.19595E-04  -0.53528
  5    tV          444.73        1.4142        4.9490       0.72693E-05
  6    kVO        0.93850       0.35649E-02   0.44751E-06    22.582
  7    nVO        0.34162E-01   0.29159E-02   0.30639E-05    2.7732
  8    tVO         51.177        1.3897       0.10498E-02   0.10383E-01

EXTERNAL ERROR MATRIX.    NDIM=  50    NPAR=  6    ERR DEF=  1.00
 0.825E-05 0.428E-06 0.284E-07-0.301E-05 0.142E-05 0.122E-02
 0.428E-06 0.258E-04-0.552E-07 0.121E-04-0.107E-04 0.293E-02
 0.284E-07-0.552E-07 0.200E+01-0.659E-07 0.515E-07 0.116E-04
-0.301E-05 0.121E-04-0.659E-07 0.127E-04-0.103E-04-0.178E-02
 0.142E-05-0.107E-04 0.515E-07-0.103E-04 0.850E-05 0.114E-02
 0.122E-02 0.293E-02 0.116E-04-0.178E-02 0.114E-02 0.193E+01
```

```
 PARAMETER  CORRELATION COEFFICIENTS
       NO.  GLOBAL     3     4     5     6     7     8
        3  0.96885  1.000 0.029 0.000-0.294 0.170 0.305
        4  0.98322  0.029 1.000 0.000 0.671-0.723 0.415
        5  0.00001  0.000 0.000 1.000 0.000 0.000 0.000
        6  0.99958 -0.294 0.671 0.000 1.000-0.990-0.358
        7  0.99944  0.170-0.723 0.000-0.990 1.000 0.280
        8  0.98222  0.305 0.415 0.000-0.358 0.280 1.000
 ENTER MINUIT COMMAND:
```

That was a little harder for minuit, but it is looking pretty good. I can now somewhat trust the ERROR values in the printout and get some meaning out of the error matrix. The correlation coefficients are really useful here. They tell me whether my fit parameters are statistically independent or correlated. For example, parameter 4 is highly correlated with itself (1.0) and parameters 6, 7, and 8. It is not very corellated with with SiO_2 thickness.

These error values from migrad assume the error surface is quadratic, which I suspect is not strictly true. Therefore, I am going to run minos to do a better estimation of the errors before I worry any more about these.

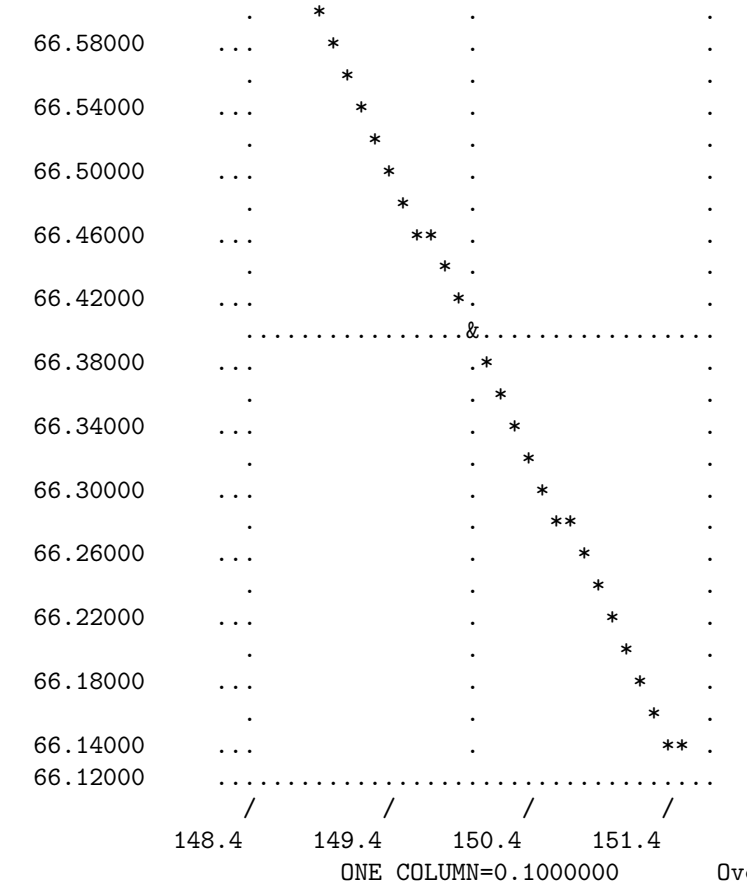
```
 ENTER MINUIT COMMAND:
minos
 **********
 **    5 **MINOS
 **********
 MINUIT WARNING IN MIGRAD
 ============== Negative diagonal element  3 in Error Matrix
 MINUIT WARNING IN MIGRAD
 ============== Negative diagonal element  4 in Error Matrix
 MINUIT WARNING IN MIGRAD
 ==============     0.10E+01 added to diagonal of error matrix
 MINUIT WARNING IN MNCROS
 ============== Cannot find slope of the right sign
                         POSITIVE MINOS ERROR NOT CALCULATED FOR PARAMETER   5

 MINUIT WARNING IN MNCROS
 ============== Cannot find slope of the right sign
                         NEGATIVE MINOS ERROR NOT CALCULATED FOR PARAMETER   5

 MINUIT WARNING IN MIGRAD
 ============== Negative diagonal element  2 in Error Matrix
 MINUIT WARNING IN MIGRAD
 ==============     0.10E+01 added to diagonal of error matrix
 EIGENVALUES OF SECOND-DERIVATIVE MATRIX:
        -0.2410E+00  0.1034E-01  0.4649E+00  0.1000E+01  0.3766E+01
```

```
 MINUIT WARNING IN MIGRAD
 ============== MATRIX FORCED POS-DEF BY ADDING  0.24478     TO DIAGONAL.

 MINUIT TASK: Example run

 FCN=   64.48379     FROM MINOS     STATUS=PROBLEMS    5039 CALLS     6062 TOTAL
                     EDM=  0.39E-05    STRATEGY= 1      ERROR MATRIX ACCURATE

  EXT PARAMETER                  PARABOLIC         MINOS ERRORS
  NO.   NAME        VALUE          ERROR      NEGATIVE      POSITIVE
   1    sigma2     0.12000E-04   constant
   2    tSiO2       18.000       constant
   3    nV         0.89796       0.28725E-02  -0.45763E-02   0.79788E-02
   4    kV         0.83976E-01   0.50808E-02  -0.98390E-02   0.14301E-01
   5    tV          444.73        1.4142
   6    kVO        0.93850       0.35649E-02  -0.58415E-02   0.80532E-02
   7    nVO        0.34162E-01   0.29159E-02  -0.53908E-02   0.41168E-02
   8    tVO         51.177        1.3897       -5.5954        8.3869
 ENTER MINUIT COMMAND:
```

This gives me the (symmetric) parabolic estimates of the errors as well as a more accurate non-linear estimate of the errors as (asymmetric) negative and positive errors.

I should note at this point, that the fit doesn't make good physical sense yet. After playing with it a little more, I got a better physical fit. The moral is, make sure you look at the fit and think about it! Don't believe whatever the program spits out.

```
 ENTER MINUIT COMMAND:
set par 5 150
 **********
 **    6 **SET PAR    5.000       150.0
 **********
 ENTER MINUIT COMMAND:
scan 5
 **********
 **    7 **SCAN    5.000
 **********

 FIRST CALL TO USER FUNCTION AT NEW START POINT, WITH IFLAG=4.
0SCAN OF PARAMETER NO.  5,  tV
   66.70000     ..................................
                  .*              .                .
   66.66000     ... *              .                .
                  .  *             .                .
   66.62000     ...   *            .                .
```




```
FCN=   66.14209     FROM SCAn      STATUS=IMPROVED      32 CALLS     6094 TOTAL
                    EDM= unknown    STRATEGY=1  ERROR MATRIX UNCERTAINTY=100.0%

 EXT PARAMETER                APPROXIMATE     INTERNAL      INTERNAL
 NO.   NAME        VALUE          ERROR       STEP SIZE       VALUE
  1    sigma2     0.12000E-04   constant
  2    tSiO2       18.000       constant
  3    nV         0.89796       0.28725E-02  -0.39445E-04   0.89796
  4    kV         0.83976E-01   0.50808E-02   0.61116E-04  -0.72628
  5    tV          151.50        1.4142      -0.79729E-03    151.50
  6    kVO        0.93850       0.35649E-02   0.46785E-04   0.93850
  7    nVO        0.34162E-01   0.29159E-02  -0.26071E-03   -1.0419
  8    tVO         51.177        1.3897        1.3897        51.177
ENTER MINUIT COMMAND:
```

After running migrad and minos on this solution, I get

```
FCN=   63.52768     FROM MINOS     STATUS=SUCCESSFUL  4187 CALLS    10783 TOTAL
```

```
                     EDM=  0.47E-05  STRATEGY=1  ERROR MATRIX UNCERTAINTY=  5.5%

  EXT PARAMETER                   PARABOLIC         MINOS ERRORS
  NO.   NAME        VALUE           ERROR      NEGATIVE      POSITIVE
   1    sigma2     0.12000E-04   constant
   2    tSiO2       18.000       constant
   3    nV         0.89783       0.45186E-02  -0.42644E-02   0.84636E-02
   4    kV         0.82797E-01   0.11630E-01  -0.10150E-01   0.16299E-01
   5    tV          186.16        33.862       -38.120        49.412
   6    kVO        0.93809       0.73638E-02  -0.60619E-02   0.84379E-02
   7    nVO        0.34549E-01   0.51141E-02  -0.56259E-02   0.42373E-02
   8    tVO         50.982        7.3566       -6.0345        9.5528
```

Now that you have a fit, save it in a disk file with the `save` command.

```
 ENTER MINUIT COMMAND:
sav
 **********
 **   10 **SAV
 **********
 UNIT  7 IS NOT OPENED.
 PLEASE GIVE FILE NAME:
101.out
 SHOULD UNIT  7 BE REWOUND BEFORE WRITING TO IT?
n
    16 RECORDS WRITTEN TO UNIT   7:101.out
 INCLUDING    4 RECORDS FOR THE COVARIANCE MATRIX.

 ENTER MINUIT COMMAND:
```

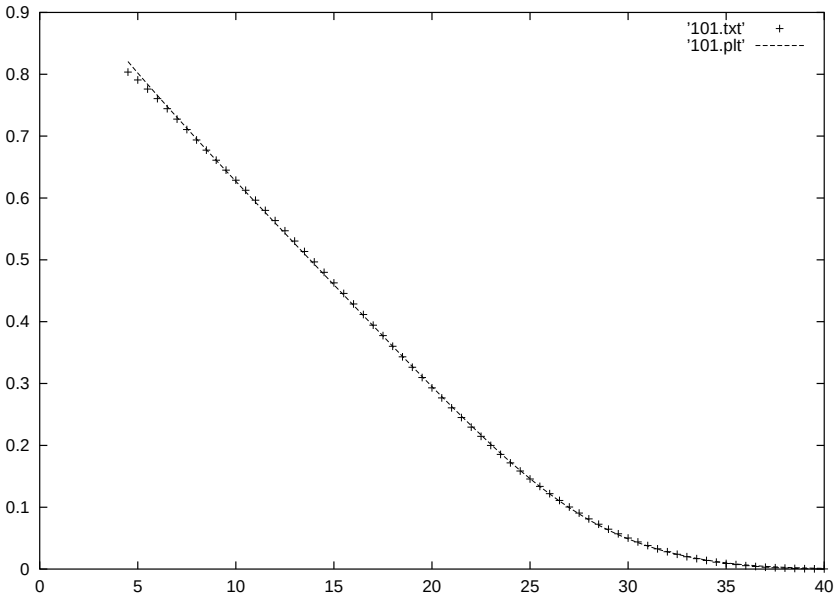
4.4 Graphing

Now we are ready to see what the fit looks like. The fitting is terminated with the `return` command.

```
 ENTER MINUIT COMMAND:
return
 **********
 **   11 **RETURN
 **********

 CALL TO USER FUNCTION WITH IFLAG = 3

plot file name: 101.plt
Hit return to continue
```

This will display a graph of the data and fit using the gnupot program. I'll let you read about gnuplot in another tutorial. For now, suffice it to say that it will

display a plot on your x-window screen until you type return. The plot from this fit is shown below.



4.5 Reflectance Theory

This section outlines the theory used int fitals program to compute the value FCN used in the minuit library. The explanation of reflectance calculations comes most immediately from Shannon Lunt's thesis.

Central to the design of mirrors in the EUV is the index of refraction. The contrast in the index of refraction between the materials used in a multilayer mirror helps determine the thicknesses of the various layers. Knowing the index of refraction well means that theory and experiment should agree rather closely. Unfortunately, this is not the case in the EUV as this region of the spectrum has not been thoroughly studied. Weaver, Henke, and Chantler have compiled tables of the optical properties of most of the elements and some compounds using various models [1, 2, 3]. Values from these and other sources do not agree and there are gaps in the EUV data where the indices of refraction of some materials have never been reported.

The complex index of refraction of a material is

$$N = n + ik \ , \tag{2}$$

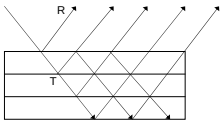


Figure 1: Reflection from Multiple Surfaces

where n is the real part of the index of refraction and k is the imaginary part or the absorption coefficient. For all materials in the EUV, the real part of the index of refraction is very close to 1, the index of vacuum. As a result, n is written as $1 - \delta$, with δ very small. The value of δ at 304 Å for molybdenum, a common material used in multilayers, is 9.5862×10^{-02} [4]. The absorption, k, in this region is fairly large and is often written as β. The value of β for molybdenum at 304 Å is 4.2986×10^{-01} [4]. This means that it is very difficult to get high reflectance from a surface in the EUV due to its low index of refraction and high absorption. In order to get higher reflectance, multilayer films are used with the result that the reflection from each surface adds, as shown in Figure 1.

Determining the order of layers and the relative thicknesses of each are some of the difficulties of making mirrors in this region. These techniques have been extensively studied and methods have been developed for theoretically designing the optimum mirror for a certain wavelength [5, 6].

4.5.1 Optical Constants - Equations

Following are equations from Spiller [5] that are useful in determining optical constants in the EUV. The imaginary index of refraction was defined in Equation 2. The index of refraction is also related to the dielectric constant, $\epsilon = \epsilon_1 + i\epsilon_2$, as follows:

$$\epsilon_1 = (1 - \delta)^2 - \beta^2 \tag{3}$$

$$\epsilon_2 = 2(1 - \delta)\beta \ . \tag{4}$$

One can use δ and β as calculated from ϵ_1 and ϵ_2 to define the atomic scattering factor, $f = f_1 - if_2$, which is related to the number of free electrons in the material. Values for f_2 can also be calculated from absorption data, as shown

in Equation 6, and f_1 is found from f_2 using Kramers-Kronig relations [10]. This calculation assumes that f_2 is known for a large number of wavelengths in order to calculate f_1. The atomic scattering factor is related to the index of refraction as follows [9]:

$$\delta = \frac{n_a r_e \lambda^2}{2\pi} f_1 \tag{5}$$

$$\beta = \frac{n_a r_e \lambda^2}{2\pi} f_2 \ , \tag{6}$$

where n_a is the atomic density, λ is the wavelength of light, and r_e is the classical electron radius defined as

$$r_e = \frac{e^2}{4\pi\epsilon_0 mc^2} \ , \tag{7}$$

which is equal to 2.82×10^{-13} cm. These equations are defined for atoms using the Drude theory. To calculate the atomic scattering factors for a compound, the density for the compound is used in place of the atomic density.

To calculate the reflectance of our films we fit the optical constants using the Fresnel coefficients, r_s and r_p. From Kohn [7] and Parratt [8], the Parratt recursion formulas allow calculation of the Fresnel coefficients for a general stack of thin layers.

$$q_i = \sqrt{n_i^2 - (\cos(\theta))^2} \tag{8}$$

$$k_{zi} = k q_i \ , \tag{9}$$

with the wave number defined as $k = \frac{2\pi}{\lambda}$. C_2 includes the phase information for the wave calculated halfway between the layers as in Figure 2:

$$C_2 = e^{ik_{z2}D_2/2} \ . \tag{10}$$

The equations for f_s and f_p are variations on the Fresnel coefficient equation:

$$f_{s2} = \frac{q_2 - q_1}{q_1 + q_2} \tag{11}$$

$$f_{p2} = \frac{n_1^2 q_2 - n_2^2 q_1}{n_1^2 q_2 + n_2^2 q_1} \tag{12}$$

These are then used to calculate the recursive Fresnel coefficients r_s and r_p:

$$r_{s2} = C_2^4 \frac{f_{s2} + r_{s1}}{1 + f_{s2} r_{s1}} \tag{13}$$

$$r_{p2} = C_2^4 \frac{f_{p2} + r_{p1}}{1 + f_{p2} r_{p1}} \ . \tag{14}$$

The actual reflectance for the sample is calculated using the coefficients for the N^{th} layer, R_s and R_p:

$$R_s = |r_{sN}|^2 \tag{15}$$

$$R_p = |r_{pN}|^2 \ . \tag{16}$$

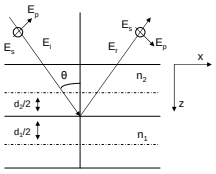


Figure 2: Geometry for Reflection Calculations

The actual reflectance is $R_s = RC^2$ but for the top layer $C = 1$. Therefore, the total reflectance of the film is found by combining R_s and R_p according to the polarization of the source. At the ALS, the source is 90% s-polarized so $R = .1R_p + .9R_s$.

4.5.2 Computing χ^2

The function FCN used in fitals is the value of χ^2 for the fit. In theory,

$$\chi^2 = \sum_{i=1}^{N} \frac{(R_i - R(n, \theta, t))^2}{\sigma_i^2} \ , \tag{17}$$

where N is the number of measured data points; R_i are the measured reflectances at each angle θ; $R(n, \theta, t)$ are the theoretical reflectances as a function of the indices of refraction n, the angle θ, and the thicknesses t of the layers; and σ_i is the uncertainty in the measurements R_i at each point. In practice, the program assumes σ^i is constant at each point and is an adjustable parameter. It should be set in the program so that χ^2 is equal to the number of data points N minus the number of parameters being fit.

5 Unix Primer

This section has instructions for connecting to volta through the computers in N212 ESC (Section 5.1) and a brief primer on unix commands (Section 5.2). It is intended to be a survival guide rather than a complete reference. Please refer to a unix book (there are several in the bookstore) and appropriate help files and man pages for further information.

5.1 Connecting to Volta

This program explains how to connect to volta from one of the Windows computers in N212 ESC. If you would like to access volta from another computer, please see me and I'll help you as best I can.

5.1.1 Establishing a Connection

1. Start x-windows client MIX by clicking on
   Start/All Programs/Microimages/MIX.
2. Start the secure shell client. This is probably on the Desktop as an icon. If it is not, click on
   Start/All Programs/SSH Secure Shell/Secure Shell Client.
3. Select Edit/Settings from the drop down menu.
4. Click on the Tunnelling selection in the left-hand pane. It is under Profile Settings/Connection.
5. In the right-hand pane, make sure the box labelled TunnelX11 Connections is checked.
6. Click OK.
7. Click on the Quick Connect menu item at the top of the window.
8. If you are prompted about whether you would like to save the current settings, click on Yes.
9. Fill in the dialog box with the host name of volta.byu.edu and your own user name (or that of the group account). If you need an account or the user name and password for the group account, give me a call or email me. Leave the other two boxes (Port Number and Authentication Method) unchanged.
10. Click the connect button.
11. Fill in your password (or the group password) in the dialog box when prompted.
12. Click OK.

13. Cancel the box asking if you want to save the connection settings.

14. You are now logged onto volta in your root directory through the secure shell client.

15. You will probably find it easiest to use volta through the x-windows interface. This gives you access to multiple windows and graphics output. To switch to the x-windows interface, type the command

    ```
    xterm &
    ```

    in the secure shell window.

16. Switch back to the MIX window (labelled MicroImages X Server).

17. Click somewhere on the screen to direct placement of the xterm window.

18. You can now type unix commands into the xterm window. A brief list of some of the commands you might find helpful is included in the next section.

A few things will help you navigate within the x-windows environment provided by MIX.

1. A window only responds to typed commands when the mouse is over the window.

2. Clicking on the top edge of a window will bring it to the top of the pile.

3. Windows can be minimized, maximized, or deleted by clicking on the controls at the upper right of the window. They have about the same meaning they do in Microsoft Windows.

4. MIX will exit when the last window is destroyed from the screen.

5.1.2 File Transfers

You can use the secure shell client to transfer files back and forth between the PC you are working on and volta. The left-hand pane will list files on the PC you can upload to volta by right-clicking on the file and selecting "upload dialog." The right-hand pane will list files on volta you can download to the PC by right-clicking on the file and selecting the "download dialog."

5.2 Unix Commands

The following commands may be helpful to you in navigating unix while analyzing data.

5.2.1 Commands

cp file1 file2 Copy file1 to file2.

lp file Print file on the printer in Dr. Turley's office. To print in the Department Office use the command `lp -d FrontOffice file`. I hope to have the printer in N212 ESC working shortly. At that point, you will be able to type `lp -d N212 file` to get a file to print there.

ls Directory listing of current directory. This command has a lot of switches for giving different formants. Type verb+man ls+ for a list of them.

man command Help (manual) on command.

mkdir newdir Make directory newdir. It can either be a subdirectory of the current directory (if it does not start with a '/') or have an absolute path name.

mv file1 file2 Rename (move) file1 to file2.

cd newdir Change directory to newdir. The directory can either by an absolute directory path (starting with a '/') or relative to the current directory.

pwd Present working directory.

rm file Delete file.

5.2.2 Files and Directories

Unix has a directory hierarchy similar to that in Microsoft Windows. All directories are relative to the root directory '/'. File reference can include the directory name to the left of the file name. For instance, I have a file in my home directory with the name `/home/turley/info.txt`. If no directory name is supplied, the file is assumed to be in your current working directory. Directory references can also be made relative to your current directory by leaving off the beginning '/'. So, for instance, if I am currently in my home directory `/home/turley` I can reference the file `fitals.f` in the directory `/home/turley/source` either as `/home/turley/source/fitals.f` or as `source/fitals.f`.

Each file and directory has three levels of permissions. You can see the permissions by typing `ls -l filename`. For instance, if I type `ls -l info.txt` from my root directory I see

```
-rw-rw-r--    1 turley   turley        510 Feb 15 13:04 info.txt
```

The information in the first column tells my what kind of file this is and which permissions each kind of user has. The first letter in the string is either a '-' or a letter specifying a special file ('d' would represent a directory, for instance). The next three letters specify the permissions for the owner of the file. They are followed by three letters with permissions for others in the same group. The final three letters are the permissions for a user who is not the owner or in the

specified group. If the letter 'r' appears in the permissions, this user can read the contents of the file. The letter 'w' signifies permission to write to the file (or delete the file). The 'x' permission is to execute the file. Permissions can be changed with unix `chmod` command (see the man page for more details).

The second column in the directory listing has the number of hard links to the file (which I won't explain here). It is followed by the name of the owner and group for the file, the number of bytes in the file, the date the file was last modified, and the full file name.

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