Index_Calc.xls Help Document

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Terminology

A "workbook" is an entire *.xls file, while a "worksheet" refers to a single sheet within such a file. "R" refers to the reflectance of a film, and "T" to the transmittance. *Solver* is a powerful numerical analysis tool that is used throughout this workbook in order to find various parameters. The word solver has been italicized in order to make it clear what is being discussed.

History

The index_calc.xls workbook started as a small template file for calculating and plotting R and T from data taken on the spectrometer system in Weniger 118. Originally, this system was only capable of measuring spectra from about 200-900nm. Prof. Janet

Tate added a few simple calculations and plots for computing the absorption coefficient (a), and band-gap. Later, a lead-sulfide (PbS) detector was added to the system to extend its range into the near-IR (~2500nm), at this point the workbook was enhanced to include the IR spectra. In this way as the spectrometer evolved so did the workbook.

When it became apparent that a method for measuring the index of refraction was needed Prof. David McIntyre began modifying the workbook. Later I enhanced, updated, made more accessible and generally re-wrote what he had started to create the workbook that exists now. Along the way, we found that it may be possible to determine the thickness of the film from our data as well.

The index_calc.xls workbook is a Microsoft Excel workbook designed to calculate the index of refraction of thin films based on reflection and transmission spectra. Originally the idea of this workbook was to create a template in which one would only need to input the raw reflection, transmission and lamp spectra, in order to calculate the index of refraction and thickness of the film. In the end I believe that the workbook achieved this goal relatively well. Although there are a few intermedia te steps before these parameters are obtained they are straight forward once you learn to navigate your way through the workbook.

Getting Started

The best way to get started using this workbook is to familiarize yourself with what each worksheet does and where the parameters are defined. The issue of becoming familiar with each worksheet is outlined below in the workbook overview section. Go to the "Help" worksheet in order to find links to the location of each parameter.

One of the most important things about this workbook is that you should never need to enter any values or data into a cell unless that cell is blue. I have labeled some boxes in green, to indicate that they are reference variables, but reference variables have no dependents, and thus should have no reason to be changed. Reference variables are placed in locations where they can be compared to other variables conveniently.

Once one has become familiar with the worksheets and parameters of this workbook, it may be instructive to begin to look at each calculation more closely. Most of the more complicated calculations are done in the calc-index, calc-n_fixed and calcn_variable worksheets. Understanding these worksheets should be done last and may require reading more literature than this document. The next section outlines each worksheet in the workbook and goes over some of the more complex worksheet functions and their uses.

Workbook Overview

Each worksheet is described below in detail. Each worksheet name (except the "Help" and "info" worksheets) has two parts. The first part tells you what type of worksheet it is; i.e. a data (dat) worksheet contains data that is obtained from an external source, a graph (gph) worksheet contains a graph, and a calculation (calc) worksheet contains calculations based on the external data and the formulas contained within the worksheet. The second part of the name further classifies what is happening in the worksheet.

I) graph-mstr – Master graph of all normalized spectra contained in worksheet

- This graph displays the Transmission, Reflection and T/(1-R) data normalized to the bare lamp.
- Transmittance spectra are in reddish colors, reflectance in blues, and T/(1-R) in greens.
- 3) The data for this graph is contained in various "dat" worksheets.
- 4) Things to watch out for:
 - A) Be sure the data range contains all of the data you want it to.
 - (i) Here and in all graphs of spectra, the data ranges are, by default, set wide so that, unless the data set is huge, all the data is plotted. If the data range does become huge, you may need to adjust it.
 - (ii) Data near either end of a spectra might be high in noise. You should cut this data from the graph by shrinking the data range appropriately.
 - (iii)To change the data range right click on the graph and select "SourceData..." then click on the "Series" tab, then click the appropriate series, and adjust its range.
- II) info This worksheet is where the film name and material of the film is placed to change the graph labels and other text boxes globally throughout the workbook.
 Also, insert the thickness measured externally here. Other plot display text is also calculated here.
 - ALWAYS BE SURE TO INPUT THE FILM NAME! The importance of this cannot be overemphasized, I recommend getting in the habit of doing this when you paste your first set of data into the workbook.

- 2) Note: the measured thickness is not used in any calculations by default (except when you use the "calc n w/ d measured" button on the calc-index worksheet). It is merely displayed throughout the workbook as a reference. However, it can be used if you wish to, its name is *d_meas*. Most calculations are done in nm, so it should be input in these units.
- 3) There is also a location where you can input the name of the data collector and relevant dates, such as the date the data was taken and the date it was analyzed. This information will appear in the upper-left hand corner of all of the graphs.
- III) Help A worksheet that contains this text file, along with tables of variable and data locations.
 - This document is placed within the workbook template for convenience and to ensure that it is not misplaced. However, if one is familiar with the workbook, it need not be included in every workbook... just DON'T DELETE THIS DOCUMENT FROM THE MASTER WORKBOOK TEMPLATE.
 - 2) Each variable and data location is hyperlinked in the table. How do you like that! Of course you can also click on the "Name Box" on the "data input bar" and scroll down to find any name you want without being in the "Help" worksheet, but there is no description. Use this table to help get you started.

IV) **gph-UV** – A graph of data taken in the UV-visible region using the silicon detector.

- 1) Often, this will be the only spectral range for which you have taken data.
- As in all graphs the data range is the most important thing to keep track of. By default the data range is set wide.
- 3) The data for this graph is contained in the "dat-UV" worksheet.

- V) **gph-IR** A graph of all data taken in the Infrared region.
 - As in all graphs the data range is the most important thing to keep track of. By default the data range is set wide.
 - 2) The data for this graph is contained in the various IR data sheets.

VI) **dat-UV**, **dat-IR1**, **dat-IR2** – Data worksheets for data collected from the UV through the visible and into the near-infrared.

- Paste the data into the appropriate worksheet in the appropriate "raw data"
 column. The best way to do this is to copy the data from the source location and then use "paste special..." from the edit menu:
 - A) Select data at source location and copy it.
 - B) Return to appropriate "dat" worksheet. Click on the cell at the top of where you want the data pasted.
 - C) Click Edit, Paste Special.
 - D) Click the "Values" radio button.
 - E) This will paste the correct values into this column without changing the formatting or deleting any comments.
- 2) Things to be careful of:
 - A) Make sure that the formulas are the same length as the data set.
 - B) By default, common wavelength values have been placed in the "wavelength" column. However, if you change the scanning increment or scan range, be sure to change these wavelength values as well.

- dat-IR1 and dat-IR2 refer to different sections of the near-IR region. They are necessary because each diffraction gratings does not span the entire region of interest.
- VII) calc-index Worksheet that calculates the index of refraction and thickness (if you want it to) of the film.
 - The first thing a person should do in this worksheet is input the locations of the fringes and determine their corresponding *m* values.
 - By looking at the various graphs of the spectrum, place the max and min points of the interference fringes in the blue part of column K with the first fringe (highest wavelength) at the top of the column.
 - If you can see the first order (highest wavelength, *m*=1) fringe than merely set *m_o*=1. Higher order (larger *m*) fringes occur at decreasing wavelength.
 - 4) However, if you cannot see the first fringe, as is generally the case. Determining the value of m_o can be more difficult.
 - A) The following relationships work as long as the index of the film is higher than the index of the substrate (which is generally the case with our films on quartz substrates).
 - (i) m = integer: maximum in T (minimum in R)
 - (ii) $m = \text{integer} + \frac{1}{2}$: minimum in T (maximum in R)
 - B) With this simplification, one should merely try different values of m_o and then look at the graph of the data points on the gph-index worksheet.
 - (i) If the set of data looks like it is curving up as λ increases than you have guessed a value of m_o too high.

- (ii) If the set of data looks like it becomes linear as λ increases and this line has negative slope than m_o is too low.
- (iii) If the set of data appears to be becoming linear as λ increases and this line has zero slope (in other words if *n* looks as though it becomes constant as λ increases) than you have guessed the correct value of m_o .
- (iv) The plot below is an example of what is discussed in parts i, ii, and iii:



Notice that the *n* axis of this plot has been magnified. The difference between the three curves will generally be greater than this and it will thus be easier to tell which value of m_o is correct. This plot is shown as an example of the worst case scenario.

(v) Note: m_o should be either an integer or half integer and which of these it should be can be determined from the relationships in part A just a few lines up. This makes determining the correct value of m_o considerably easier. 5) The worksheet then calculates the index at that fringe according to the following equation:

$$n = \frac{m \cdot \mathbf{l}}{2 \cdot d}$$

Where *m* is the fringe number talked about above, I is the wavelength of the fringe and *d* is the thickness of the film in the same units as I. This is repeated for each fringe and these data points are displayed in the table labeled "input of fringe max/min points and associated calculations".

- 6) Before doing anything else, be sure to set up the fit range and reference page:
 - A) Look at the experimental reflectance data and determine a fit range. Here are some basic guidelines:
 - (i) Generally the upper bound of the fit range will be the upper limit of the data set in the *reference_page*. i.e. if your data goes from 200-900nm, your upper bound will be 900nm. However, if one does wish to fit the data less strongly to this part of the spectrum that is totally reasonable.
 - (ii) The lower bound of your fit should be a bit above the band gap. If a fringe or two exist in the band gap it is probably best to not include these in the fit range.
 - B) Return to the calc-index worksheet.
 - C) Input the values for the fit range in their proper locations.
 - D) Type the name of the reference worksheet that contains the experimental data you are fitting to.

- All data entry for this worksheet is essentially done. Now all that we need to do is perform the calculations necessary in determining the information we seek.
- 8) When the film thickness is not known beforehand: calculating the thickness, d, and the refractive index, n. Be sure that you have set up the fit range correctly as described above and then click the "calc n&d" button in order to begin the process.
 - A) The first thing that the "calc_n&d" button does is obtain an approximate value of the thickness. It does this by adjusting *d* in order to fit a theoretical reflectance curve to the experimental one. However, a form of the refractive index is needed. This initial form is the simple approximation to the Sellmeier equation:

$$n = int + slp \cdot 1/l^2$$

This simple form comes from a linear regression fit of n vs $1/\lambda^2$. The data points used come from the location of the fringes as discussed above. This simple form is used because its parameters can be determined without the *solver*.

- (i) Chi_2_1 is the variable that defines the error in between the theoretical and experimental reflectance spectra.
- B) Now that a value of the thickness, *d*, has been found, *solver* adjusts the parameters of the Sellmeier equation to fit the parameters of the Sellmeier equation to the set of data points for *n*. The approximation (whose derivation can be found in my thesis in the section on Refractive Index [Ref. 1]) to the

Sellmeier equation used here is:

$$n \cong \sqrt{A + \frac{l^2 \cdot G_g}{l^2 - l_g^2}} \qquad A = 1 + \sum_b G_b$$

In this second stage, *solver* adjusts the parameters A, G_g and λ_g in order to fit the equation above to the data points obtained from the location of the fringes and the previously determined film thickness.

- C) Now that we have a more exact form of the refractive index, *solver* is used to re-adjust the thickness to fit a new reflectance spectrum (which uses this more exact index) to the experimental data.
 - (i) Chi_2_2 is the error between the theoretical and experimental reflectance spectra over the fit range. In other words, it is what *solver* tries to minimize.
- D) Finally, with this more exact value of the thickness, *solver* once again fits the Sellmeier equation to the index data points (which have changed because *d* has changed) in order to determine a final approximation of the refractive index.
- E) One might think that the iterations performed in parts C and D above could be repeated indefinitely. However, if they are repeated the solution diverges from, rather converge to the correct answer. This is why I have done this many iterations and not more.
- 9) When the film thickness is known beforehand: calculating the refractive index, n.
 Click the "calc n w/ d_measured" button in order to begin the process. This will do two things:

- A) First this will set the thickness variable, d, equal to the measured thickness, d_meas, defined on the info page. Because of this, one must have a measured thickness in the appropriate cell in the info worksheet.
- B) Second, this will fit the parameters of the Sellmeier equation defined above to the data points using the *solver* to produce a functional form of the refractive index.
 - (i) Chi_2_2 is the error between the theoretical and experimental reflectance spectra over the fit range.
- 10) It is also possible to calculate the refractive index based on an arbitrary thickness or guess. To do this simply put your guess of the thickness into the thickness cell and click "calc n w/ arbitrary d". This will merely fit the Sellmeier parameters to the data points determined by this value of *d*.
- 11) Adjust the *reference_page* and fit range (*fitr_min* and *fitr_max*) in this worksheet as well.
 - A) The *reference_page* (reference worksheet) name is the worksheet which contains the data that you wish to fit the theoretical spectrum to. All that one must do is change the value of this cell (calc-index!G3) so that it matches the name of the worksheet to which you want to compare your theoretical data.
 All values within the calc-R_n-Sellmeier and calc-R_n-simple worksheets will adjust to this new reference worksheet.
 - B) Only dat-UV, dat-IR1 and dat-IR2 are valid entries for the reference page cell.
 - C) In general, you will fit the data to the UV-visible data, and so the worksheet is set to dat-UV by default.

- D) Adjust the fit range, in nm, so that it extends over most of the fringes, and not into the region of the band gap.
- E) The *delta_lambda* name is also defined in this worksheet. It is simply the increment in wavelength of the data set. It is used to calculate the fit range in column Z. It is necessary because the wavelength increment is not necessarily lnm.
- 12) The parameters A_sell , G_sell , and lambda0 correspond to the parameters A, G_g and I_g , respectively, in the Sellmeier equation defined in part VII.7.B above. In general you should not need to change them manually, but they could be changed without creating problems (*solver* will just change them back to whatever they should be). The one time one might want to change them occurs when:
 - A) Sometimes *solver* will converge on a local minimum when obtaining the parameters of the Sellmeier equation rather than the true minimum. If this happens I recommend that you put in a value for lambda0 (λ_g) that corresponds to the location of the band gap. If the problem persists, use common values for *G* and *A* such as: 1<*A*<10 and 0<*G*<10.
- 13) At the far right of the worksheet, the refractive index is calculated based on the simple $(1/\lambda^2)$ form of the index and the more complicated Sellmeier form from 0.2 to 2.0 microns so that it can be plotted in the worksheet "gph-index".
- VIII) **gph-index** Graph of index as a function of wavelength.
 - 1) This worksheet plots the index as a function of wavelength (?) for the calculations based on the fixed fringe locations *and* the *solver* solution.

- IX) calc-R_n-Sellmeier This worksheet calculates a theoretical transmittance and reflectance based on the Sellmeier equation form of the index. This calculated spectrum can then be fit to the experimental data by adjusting the thickness parameter *d* in order to obtain a value for *d*, as described in the section about the calc-index worksheet.
 - Before doing anything else, drag all formulas on this worksheet so that they are the same length as those in the reference worksheet (see below).
 - A) In the upper left hand corner, the parameters of the Sellmeier equation are displayed for convenience along with the sum of χ^2 which indicates the error between the theoretical and experimental data
 - 2) Below is a column by column record of the equations in this worksheet. Here is a diagram of a film stacked on a substrate and some labels that will clarify some of the notation:



A) Column A uses the "concatenate" function followed by the "indirect"

function. Concatenate is a function that "joins several text strings into one text string" [Ref. 2]. Here it is used to create a text form of the location of the wavelength data in column A of the *reference_page*. The "indirect" function returns the reference indicated by a text string. This simply links this cell to the reference indicated by the joined text. The concatenate and indirect worksheet functions are used together repeatedly in this worksheet.

- B) Column B is just the wavelength in column A converted to μ m.
- C) Column C is the energy in electron-volts of columns A and B.
- D) Column D is the index of refraction of quartz as a function of wavelengthThis column uses the Sellmeier equation with the following constants:

$$n = \sqrt{1 + \sum_{k} \frac{\mathbf{l}^2 \cdot G_k}{\mathbf{l}^2 - \mathbf{l}_k^2}} \qquad \qquad G_1 = 0.6962 \qquad \mathbf{l}_1 = 0.0684 \, \mathbf{m}n$$
$$G_2 = 0.40794 \qquad \mathbf{l}_2 = 0.11624 \, \mathbf{m}n$$
$$G_3 = 0.89748 \qquad \mathbf{l}_3 = 9.89616 \, \mathbf{m}n$$

Here λ is in μ m.

- E) Concatenate and indirect are again used to link this column to the column containing the T/(1-R) data in the *reference_page* worksheet.
- F) This is simply the index of refraction of the film as determined by fitting coefficients of the Sellmeier equation to the index at the fringe locations.
- G) This is the normal incidence reflection coefficient at the film-substrate interface according to the below equation where n_f is the index of the film and n_s is the index of the substrate. Note that in the r_{ab} notation the beam is incident on medium b and reflected in medium a.

$$r_{fs} = \frac{n_f - n_s}{n_f + n_s}$$

H) Here, an intermediate variable of the absorption coefficient, x, is calculated that takes complex interference effects of the film into account.

$$x = \left(\frac{T}{1-R}\right)^{1-\left(\frac{T}{1-R}\right)^{2}} r_{fs}^{2}} = e^{ad}$$

I) In column I α , the absorption coefficient, is calculated from the intermediate variable, x in column H according to the equation:

$$a = \frac{\ln(x)}{d}$$

 J) Here the imaginary part of the complex index, k, is calculate from alpha according to:

$$k = \frac{\boldsymbol{a} \cdot \boldsymbol{l}}{4\boldsymbol{p}}$$

- K) In column K, the complex index, n_cmplx, is created from k and the real part of the index, n.
- L) The next few columns (L-S) simply calculate the reflection and transmission coefficients for each interface using the normal-incidence fresnel equations. The notation in the diagram above, as used by Hishikawa et. al. [Ref. 3], is used here to label each column. Where r_{ab} is the reflection coefficient of light incident on material b and reflected in material a. And t_{ab} is the transmission coefficient from material a into material b.

$$r_{ab} = -r_{ba} = \frac{n_a - n_b}{n_a + n_b} \qquad t_{ab} = \frac{2 \cdot n_a}{n_a + n_b}$$

T) Column T is an intermediate exponential variable. In Hishikawa [Ref. 3], it is labeled e_1 , and so I use this notation here.

$$e_1 = e^{\frac{i \cdot 2\mathbf{p} \cdot n_cmplx \cdot d}{\mathbf{l}}}$$

U) The next set of columns calculate transmittance and reflectance for various stacks. The equations are straight out of Hishikawa et al. [Ref. 3]. The notation T_{ab} is the transmittance from layer *a* through all intermediate layers to layer *b*, and R_{ab} is the reflectance off of all interfaces between layer *a* and layer *b*. Column U calculates the reflectance, R, of the films interfaces only:

$$R_{02} = \left| r_{01} + \frac{e_1^2 \cdot t_{01} \cdot t_{10} \cdot r_{12}}{1 - e_1^2 \cdot r_{12} \cdot r_{10}} \right|^2$$

V) Column V calculates the reflectance backwards through the film interfaces:

$$R_{20} = \left| r_{21} + \frac{e_1^2 \cdot t_{21} \cdot t_{12} \cdot r_{10}}{1 - e_1^2 \cdot r_{12} \cdot r_{10}} \right|^2$$

W) Column W calculates the transmittance through the film interfaces:

$$T_{02} = T_{20} = \frac{n_2}{n_0} \left| \frac{e_1^2 \cdot t_{01} \cdot t_{12}}{1 - e_1^2 \cdot r_{12} \cdot r_{10}} \right|^2$$

X) This column is the calculated reflectance from the entire stack (R_{03}), and is again taken from Hishikawa et. al.

$$R = \frac{T_{20}^2 \cdot R_{23}}{1 - R_{20} \cdot R_{23}} + R_{02}$$

- Y) This column uses the concatenate and indirect worksheet functions again to obtain the experimental reflectance data from the *reference_page* worksheet. It is used to compare to the above calculated total reflectance.
- Z) This column is simply the χ^2 error of the data from the theoretical value. At the top of this column, a sum of this error is calculated over the fit range specified by the user. The concatenate and indirect functions are again used to establish the fit range based on the fit range parameters defined in this page.
- AA) Here, the total transmittance through the stack is calculated according to the equation in Hishikawa et. al.:

$$T = \frac{T_{23} \cdot T_{02}}{1 - R_{20} \cdot R_{23}}$$

- BB) Column AB is the experimental transmittance once again using concatenate and indirect. It is here to be plotted and compared to the theoretical values. Note: there is no χ^2 value calculated for the transmittance as there was for the reflectance.
- IX) calc-R_n-simple This worksheet calculates a theoretical transmittance and reflectance based on the simple form of the refractive index. This calculated spectrum can then be fit to the experimental data by adjusting the thickness parameter *d* in order to obtain a value for *d*, as described in the section about the calc-index worksheet. *Slope* and *intercept* are the variables that define the index of refraction according to the equation:

$$n = intercept + slope \cdot \frac{1}{l^2}$$

- Before doing anything else, drag all formulas on this worksheet so that they are the same length as those in the reference worksheet.
- 2) The calculations performed on this worksheet are exactly the same as those in the calc-n_fixed worksheet except that the index of refraction, *n*, in column F is determined by the simple form of the index rather than the more complicated Sellmeier form.

XI) **gph-fit_R** – Graph of the experimental and theoretical reflectance.

- 1) This worksheet is used to look and see how good the fit is.
- As usual make sure that the plot range as defined in source data is correct for the data set you are looking at.
- 3) Generally the amplitude of the theoretical fringes will be larger than the experimental ones. However, we do hope that the fringes line up with one another, if they do I believe it should be considered a decent fit.

XII) $gph-fit_T$ – Graph of the experimental and theoretical transmittance.

- This worksheet is constructed simply so that one can see how well the calculated transmittance compares to the experimental.
- 2) Again, the plot range must be correct for the data set.
- 3) Generally this plot will look better than the reflectance plot, but remember that the transmittance spectra is not used to fit the data.
- XIII) calc-gap This worksheet does some simple calculations to help determine the band gap and aborption coefficient of the material.
 - The values to which these calculations are done come from the *reference_page* worksheet as defined in the calc-index worksheet. In general this should be over

the UV-visible range. If it is not you will need to change the ranges on the gphalpha and gph-gap worksheets.

- This data doesn't mean anything unless one has both reflectance, R and transmittance, T, experimental spectra in the reference worksheet.
- 3) The d_cm name is defined and is used here in these calculations. By default it is linked to the d_nm1 name, but this can be changed to be any thickness value that you have for the film. Just be sure that the units are in centimeters.
- The alpha and wavelength data come straight from the calc-n_fixed worksheet. The gap calculations are then done based on this.
- 5) The gap calculations are for the gph-gap worksheet. There is nothing in this worksheet that says "this is the gap". Instead, one looks at the gph-gap worksheet and attempts to determine where the gap is (see the section on the gph-gap worksheet for more info.)

XIV) **gph-alpha** – Graph of the absorption coefficient, α , as a function of energy.

- This graph is an approximate graph of the absorption coefficient. There are two curves, but it is the same data, one is a linear and the other a logarithmic vertical scale.
- As in all graphs, one should make sure that the source data plot range is correct.
 Furthermore, one should also be sure that the horizontal scale is correct.

XV) **gph-gap** – Graph that can be used in determining the band gap of a material.

 This graph has two plots. One is used to determine the direct band gap, and the other to determine the indirect gap. A) The data for the direct gap plot is the determined from the following equation:

$$data = (\boldsymbol{a}(\boldsymbol{l}) \cdot \boldsymbol{E}(\boldsymbol{l}))^2$$

Where alpha is the absorption coefficient as a function of wavelength and E is the energy of a photon at that wavelength, $E = h \cdot c/I \approx 1240 nm \cdot eV/I$.

B) The data for the second plot is determined from this equation:

$$data = \sqrt{\boldsymbol{a}(\boldsymbol{l}) \cdot \boldsymbol{E}(\boldsymbol{l})}$$

C) Both of these plots are plotted as a function of energy.

2) In order to determine the gap of the material, one simply looks at the plot and attempts to see the regions where the data is linear. Then a line is drawn through this linear region, and the point where this lines intersects the horizontal axis is considered the band-gap. Sometimes there is more than one linear region on each curve, and this may indicate more than one gap. Lines drawn based on the indirect gap data correspond to indirect gaps, and lines drawn for the direct gap data correspond to direct gaps. Here is a picture of these calculations being done:





Interestingly in this case, the lines based on the indirect gap data seem to intersect at approximately the same point on the horizontal axis, where as the lines drawn based on the direct gap data have two distinct intersection points.

References

1) Kilcher, "Optical Spectroscopy of Transparent Conducting Oxides from the UV to near-IR and a Method for Determining the Refractive Index of Transparent Thin Films", (June 2003).

2) Microsoft excel help.

3) Hishikawa, Nakamura, Tsuda, Nakano, Kishi and Kuwano "Interference-Free Determination of the Optical Absorption Coefficient and the Optical Gap of Amorphous Silicon Thin Films" Japanes Journal of Applied Physics vol. 30 No. 5, May 1991 pp 1008-1014.