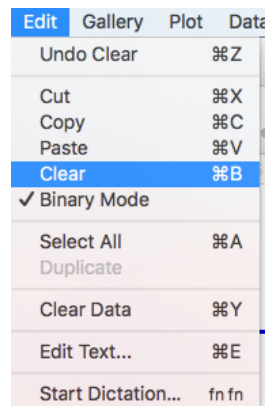


## Lesson 5\_Intermediate Curve fitting and taking a numerical derivative

Goal: to use the general curve fit feature and to be able to use the Macro menu to take a derivative.

- 1) Open the plot resulting from Lesson 4.
- 2) Erase the masked data. Do this by extracting the data from the plot by clicking on the gridiron in the upper right of the plot (as was done in a previous lesson). Click on the first row of the masked data and shift-click on the last row of the masked data and select clear from the edit pull down menu



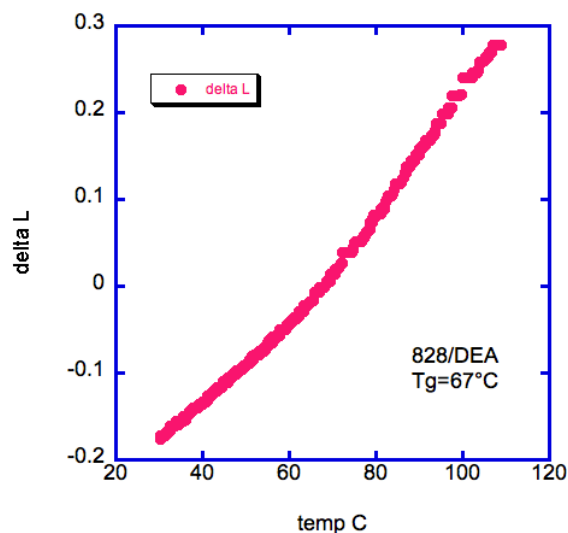
ThermalExpansion 5:56:43 PM 11/20/15

|    | time s | g p dyn/cm2 | g dp d/cm2  | tan delta | temp C | delta L   | stress .../cm2 |
|----|--------|-------------|-------------|-----------|--------|-----------|----------------|
| 0  | 12.000 | -8.5431e+08 | -6.7225e+08 | 0.78689   | 110.30 | -0.080999 | 15.972         |
| 1  | 21.000 | 3.2344e+07  | -1.1693e+08 | -3.6153   | 110.41 | -0.080999 | 2.5971         |
| 2  | 34.000 | -2.8314e+08 | -5.8500e+08 | 2.0662    | 110.45 | -0.035999 | 11.539         |
| 3  | 47.000 | -3.3673e+09 | -1.9782e+09 | 0.58747   | 110.43 | -0.035999 | 7.6127         |
| 4  | 64.000 | -8.2066e+07 | 2.0736e+08  | -2.5268   | 110.39 | -0.035999 | 7.1203         |
| 5  | 76.000 | -3.8238e+08 | 1.0354e+08  | -0.27079  | 110.34 | -0.035999 | 3.6590         |
| 6  | 85.000 | -3.5072e+08 | -2.0749e+08 | 0.59160   | 110.30 | -0.035999 | 9.4761         |
| 7  | 94.000 | -4.2624e+08 | -2.9607e+08 | 0.69462   | 110.31 | -0.035999 | 6.5581         |
| 8  | 103.00 | -2.9545e+08 | -1.2634e+08 | 0.42760   | 110.28 | -0.035999 | 7.3594         |
| 9  | 112.00 | -8.5758e+08 | 1.1663e+09  | -1.3600   | 110.26 | -0.035999 | 7.9876         |
| 10 | 121.00 | -8.5114e+08 | 2.5159e+08  | -0.29559  | 110.24 | -0.035999 | 8.6286         |
| 11 | 130.00 | 1.7205e+08  | 3.1980e+08  | 1.8588    | 110.19 | -0.035999 | 5.8719         |

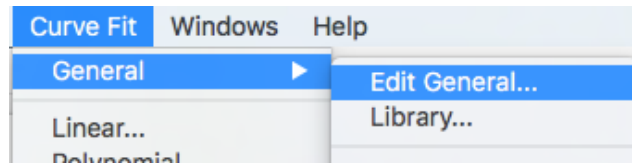
ThermalExpansion 5:56:43 PM 11/20/15

|    | time s | g p dyn/cm2 | g dp d/cm2  | tan delta | temp C | delta L | stress .../cm2 |
|----|--------|-------------|-------------|-----------|--------|---------|----------------|
| 0  | 992.00 | -3.0487e+08 | -5.8517e+08 | 1.9194    | 108.83 | 0.27800 | 7.9425         |
| 1  | 1001.0 | -2.6563e+08 | -2.9900e+08 | 1.1256    | 108.68 | 0.27800 | 3.2333         |
| 2  | 1010.0 | 2.1496e+07  | 5.4838e+08  | 25.511    | 108.52 | 0.27800 | 2.4062         |
| 3  | 1019.0 | -2.3637e+09 | 8.7759e+07  | -0.037128 | 108.37 | 0.27800 | 4.1774         |
| 4  | 1028.0 | -3.5568e+07 | 6.4434e+08  | -18.115   | 108.21 | 0.27800 | 5.0301         |
| 5  | 1037.0 | -1.0574e+09 | -4.7271e+08 | 0.44705   | 108.08 | 0.27800 | 15.507         |
| 6  | 1046.0 | 3.4168e+09  | -1.7106e+09 | -0.50065  | 107.92 | 0.27800 | 6.2818         |
| 7  | 1055.0 | 1.2058e+08  | -7.7848e+08 | -6.4558   | 107.77 | 0.27800 | 13.870         |
| 8  | 1064.0 | -4.3225e+08 | -1.0482e+08 | 0.24251   | 107.61 | 0.27800 | 9.4135         |
| 9  | 1073.0 | -5.4181e+08 | -9.2371e+08 | 1.7049    | 107.47 | 0.27800 | 7.4812         |
| 10 | 1082.0 | -1.1495e+09 | 1.2446e+09  | -1.0827   | 107.31 | 0.27800 | 8.3184         |
| 11 | 1091.0 | -2.0613e+08 | -2.3721e+08 | 1.1508    | 107.17 | 0.27800 | 6.9624         |

- 3) Delete the trend lines (click on a line and hit the delete key)

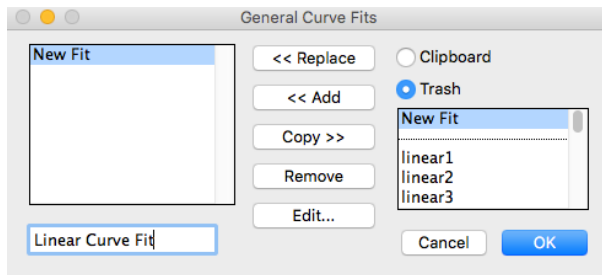


4) With the plot selected (and not the data window), select Curvefit->General->Edit General

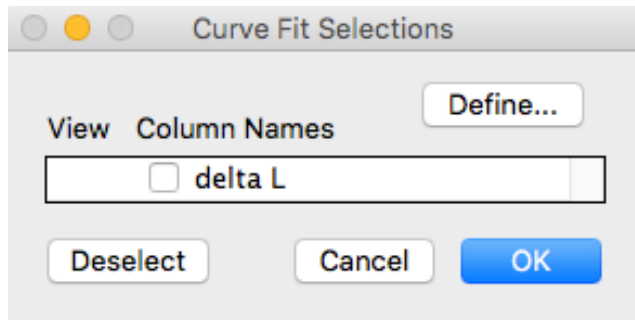
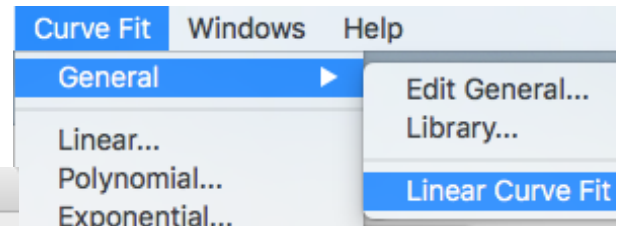


5) Select New Fit and click Add

Select New Fit and type in Linear curve fit and click OK



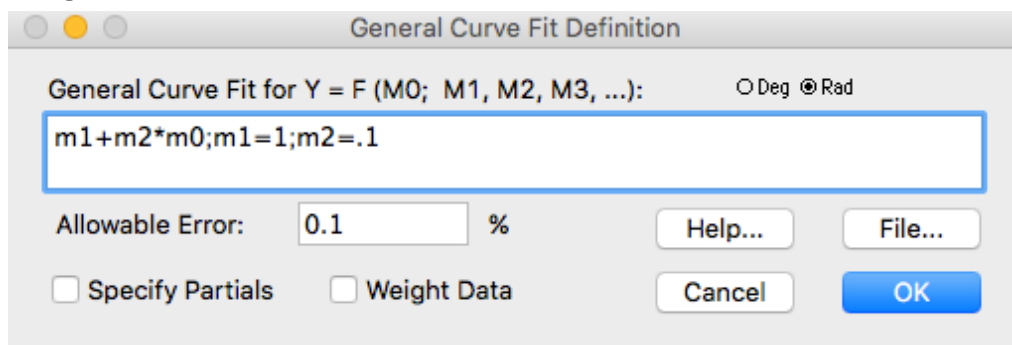
6) Select Curve fit-> General -> Linear Curve Fit



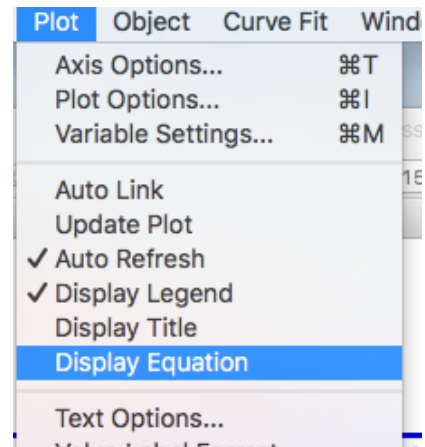
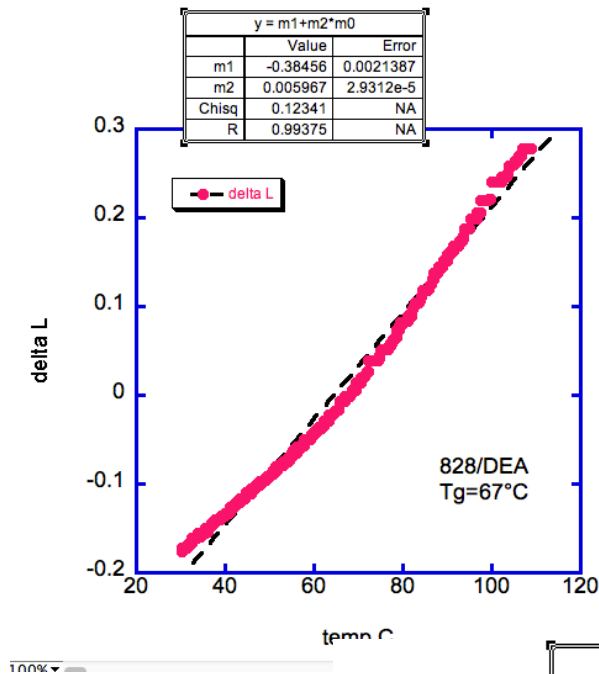
Select delta L and click "Define"

Type "m1+m2\*m0;m1=1;m2=0.1"

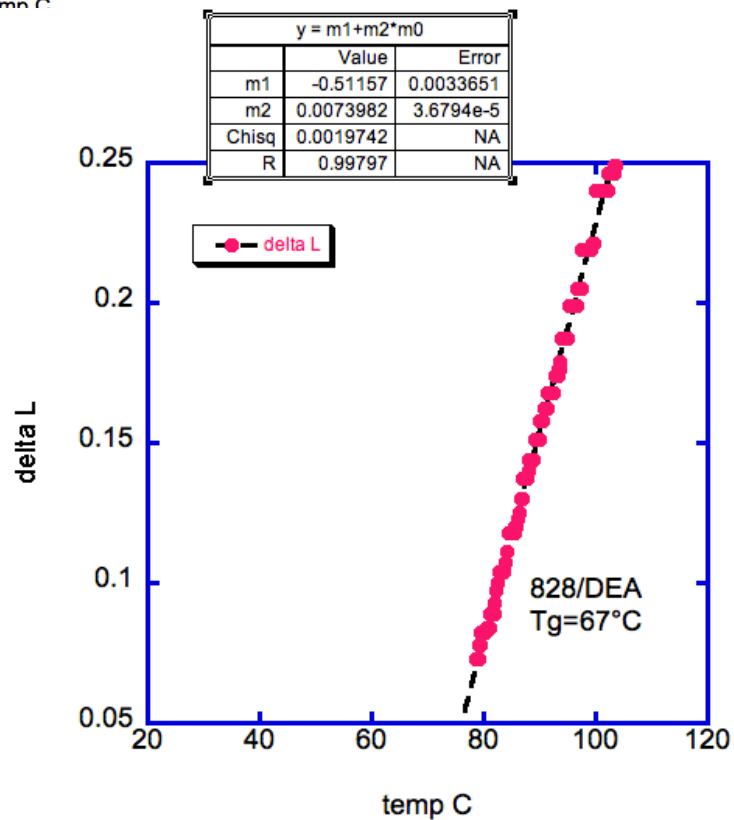
m1 and m2 are curve fit parameters and m0 is the X in the plot (temperature in this case). The ;m1=1;m2=0.1 are initial guesses of the parameters. Select OK and then OK again.



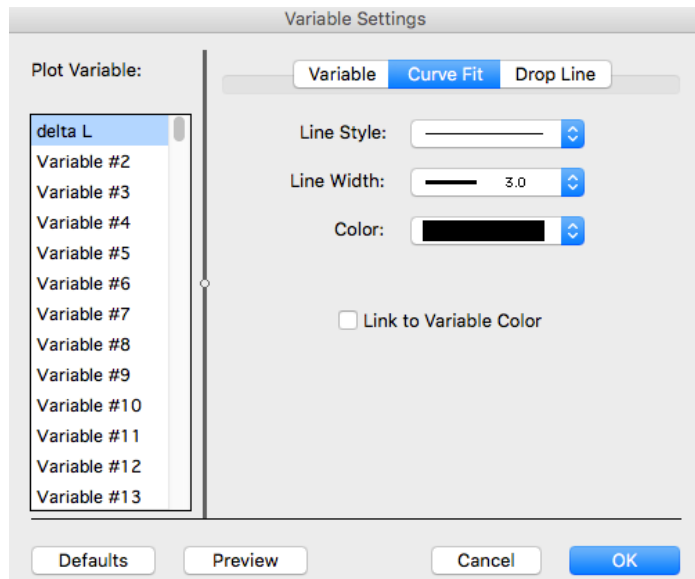
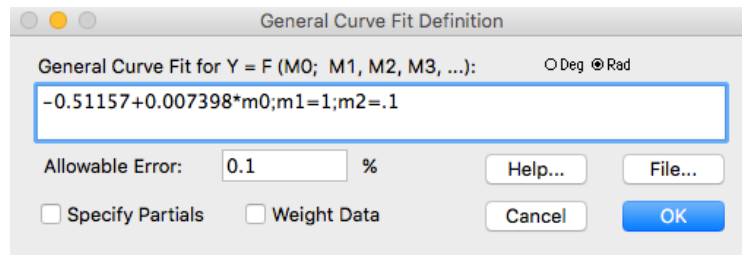
7) Select Plot->display equation and drag the equation off to the side



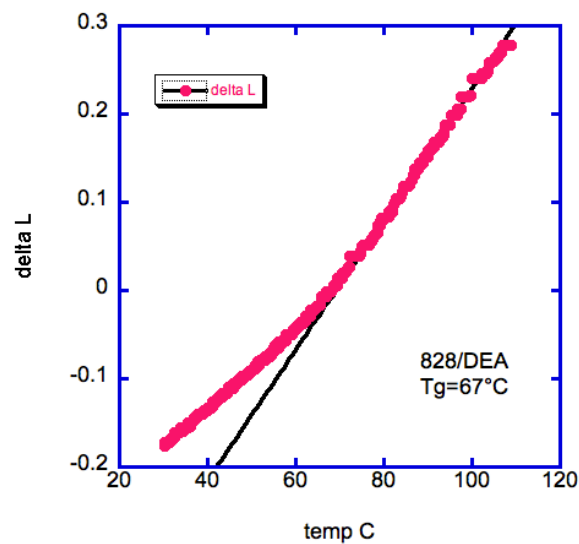
8) Mask all but the upper part of the curve.



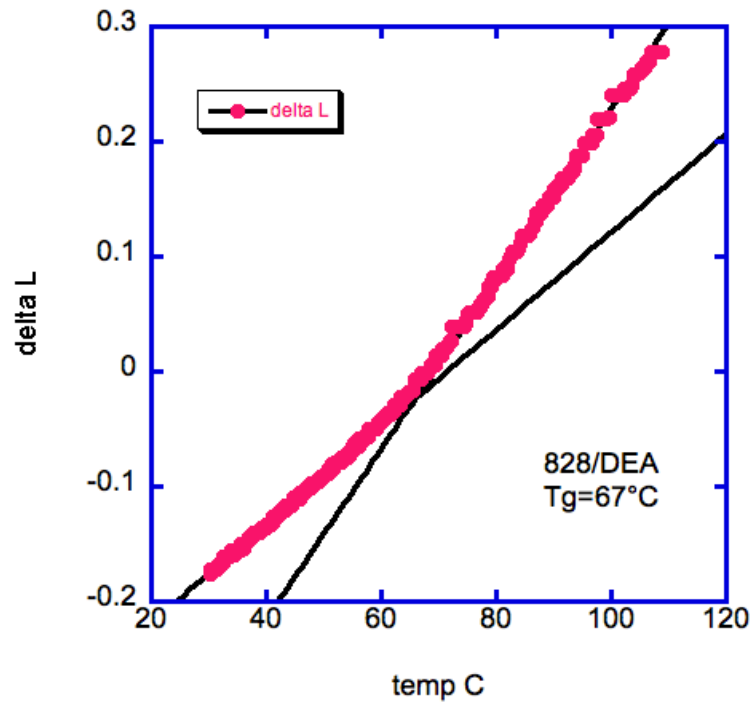
9) Select Curvefit->General->General Curve Fit and enter the m1 and m2 from the curve fit (to “hardwire” the fit) and hit ok. Also change the curve fit line into a solid line. Then double click on the mask tool to unmask the data



|                            |         |       |
|----------------------------|---------|-------|
| $y = -0.51157+0.007398*m0$ |         |       |
|                            | Value   | Error |
| Chisq                      | 1.0933  | NA    |
| R                          | 0.94318 | NA    |



10) Create a second Curve Fit (Linear Curvefit 2) and repeat the above pocedure for the low T points. Erase the displayed equations (click on them and hit delete key)



11) take the derivative to get function proportional to linear expansion coefficient. Turn off curve fits and extract data (with gridiron) and turn on column numbers. With the data window selected, choose Macros-> derivative. Put the column numbers for x and y in the prompt window and select a new output column (7)

**Prompt**

Derivative:

X Column: 4

Y Column: 5

Output Column: 7

Cancel OK

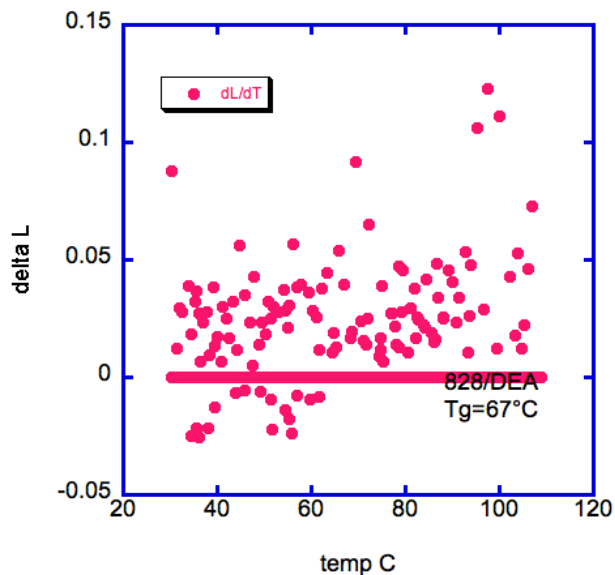
ThermalExpansion 8:04:32 PM 11/20/15

|   | g p dyn/cm2<br>C1 | g dp d/cm2<br>C2 | tan delta<br>C3 | temp C<br>C4 | delta L<br>C5 | stress .../cm2<br>C6 | dL/dT<br>C7 |
|---|-------------------|------------------|-----------------|--------------|---------------|----------------------|-------------|
| 0 | -3.0487e+08       | -5.8517e+08      | 1.9194          | 108.83       | 0.27800       | 7.9425               | 0.0000      |
| 1 | -2.6563e+08       | -2.9900e+08      | 1.1256          | 108.68       | 0.27800       | 3.2333               | 0.0000      |
| 2 | 2.1496e+07        | 5.4838e+08       | 25.511          | 108.52       | 0.27800       | 2.4062               | 0.0000      |
| 3 | -2.3637e+09       | 8.7759e+07       | -0.037128       | 108.37       | 0.27800       | 4.1774               | 0.0000      |
| 4 | -3.5568e+07       | 6.4434e+08       | -18.115         | 108.21       | 0.27800       | 5.0301               | 0.0000      |
| 5 | -1.0574e+09       | -4.7271e+08      | 0.44705         | 108.08       | 0.27800       | 15.507               | 0.0000      |
| 6 | 3.4168e+09        | -1.7106e+09      | -0.50065        | 107.92       | 0.27800       | 6.2818               | 0.0000      |
| 7 | 1.2058e+08        | -7.7848e+08      | -6.4558         | 107.77       | 0.27800       | 13.870               | 0.0000      |
| 8 | -4.3225e+08       | -1.0482e+09      | 0.24251         | 107.61       | 0.27800       | 9.4135               | 0.0000      |
| 9 | -5.4181e+08       | -9.2371e+08      | 1.7049          | 107.47       | 0.27800       | 7.4812               | 0.0000      |

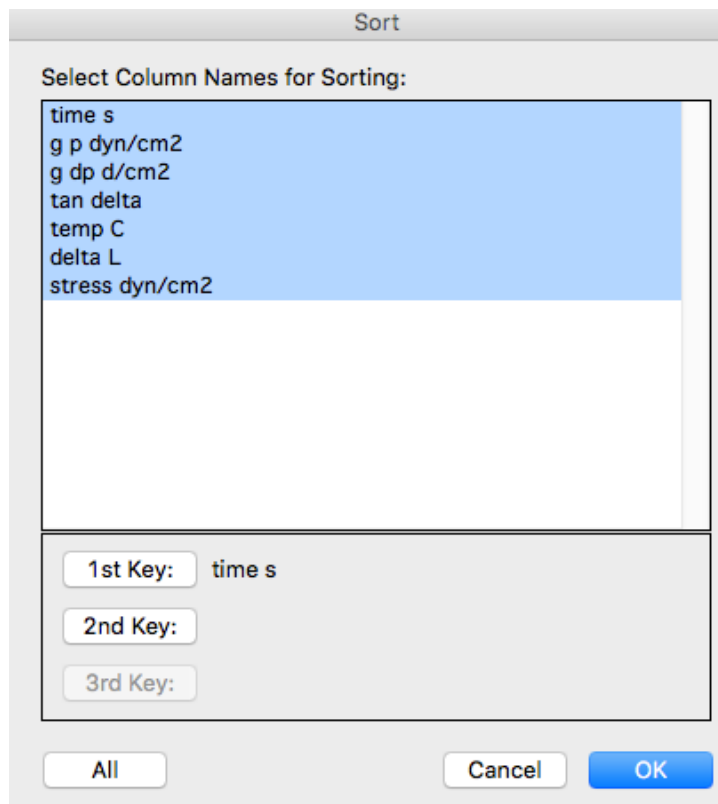
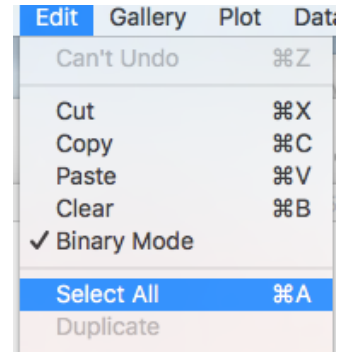
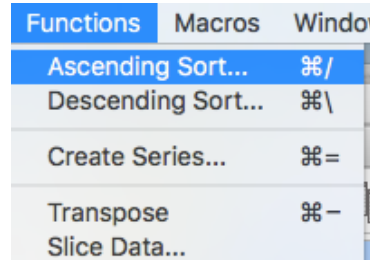
**Macros Windows**

- Show Macros...
- Library...
- Filter
- Smooth
- Simplify
- Invert Mask
- Integrate - Area
- Integral - Curve
- Derivative**
- Series
- Unit Series
- π Series
- sinc(5x)
- abs(x)
- Random#

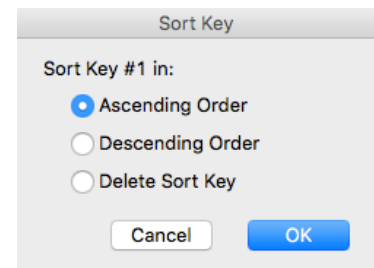
Create a New Plot of  $dL/dT$  vs. T. The result is just noise! This is an illustration of how numerical derivatives amplify noise. In order to get a meaningful derivative, the data must be smoothed before the derivative is taken.



12) For this data, the “smooth” curvefit works ok, however, the data needs to be sorted first. Go back to the previous L vs. T plot and extract the data. In the data window select all the data. Select Functions-> Ascending Sort



Click “1<sup>st</sup> Key”. Select Delete Sort Key and click OK



13) select temp C and click 1<sup>st</sup> Key. Select Ascending Sort and click OK

Select Column Names for Sorting:

|                |
|----------------|
| time s         |
| g p dyn/cm2    |
| g dp d/cm2     |
| tan delta      |
| temp C         |
| delta L        |
| stress dyn/cm2 |

1st Key:

2nd Key:

3rd Key:

All Cancel OK

14) Select all and click OK

Sort

Select Column Names for Sorting:

|                |
|----------------|
| time s         |
| g p dyn/cm2    |
| g dp d/cm2     |
| tan delta      |
| temp C         |
| delta L        |
| stress dyn/cm2 |

1st Key: temp C

2nd Key:

3rd Key:

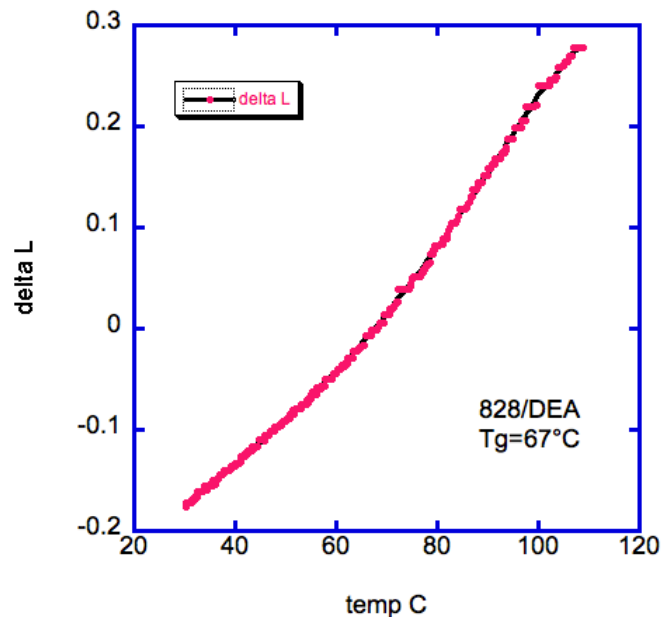
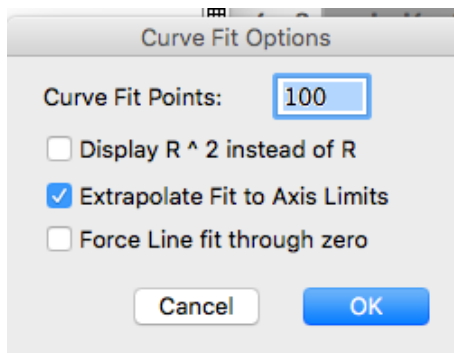
All Cancel OK



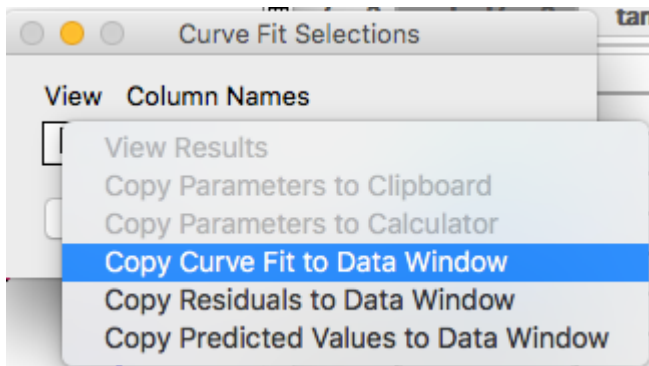
15) click on the data window so the data becomes unselected. You should now see:

|   | time s | g p dyn/cm2 | g dp d/cm2  | tan delta | temp C | delta L  | stress .../cm2 |
|---|--------|-------------|-------------|-----------|--------|----------|----------------|
| 0 | 5736.0 | -2.6189e+08 | 8.0607e+08  | -3.0779   | 30.183 | -0.17700 | 16.973         |
| 1 | 5727.0 | 1.9357e+08  | -1.2217e+09 | -6.3113   | 30.240 | -0.17200 | 8.6209         |
| 2 | 5718.0 | -1.5685e+09 | 4.8950e+08  | -0.31208  | 30.301 | -0.17200 | 11.041         |
| 3 | 5709.0 | -7.1448e+08 | 2.5245e+08  | -0.35332  | 30.387 | -0.17200 | 15.123         |
| 4 | 5700.0 | -1.3806e+08 | 6.3613e+08  | -4.6075   | 30.467 | -0.17200 | 13.374         |
| 5 | 5691.0 | -3.4596e+08 | 3.4576e+07  | -0.099942 | 30.553 | -0.17200 | 3.1170         |
| 6 | 5682.0 | -1.8423e+09 | 1.3350e+09  | -0.72466  | 30.660 | -0.17200 | 29.127         |
| 7 | 5673.0 | -3.3932e+07 | 1.9456e+08  | -5.7338   | 30.783 | -0.17200 | 2.8029         |
| 8 | 5664.0 | -7.2027e+08 | 6.7588e+07  | -0.093837 | 30.915 | -0.17200 | 9.5933         |
| 9 | 5655.0 | -1.4108e+09 | -2.8059e+08 | 0.19889   | 31.072 | -0.17200 | 19.425         |

16) We are now ready to do a curve fit. Click on the plot to bring it to the foreground and select Curvefit-> smooth and then select curvefit-> curvefit options. Change the Curve fit points to 1000 and click OK. Reduce the point size for the red data to 9 pt



17) Select Curve fit-> Smooth and copy curve fit to data window



18) There should now be two new columns in the data window with the T (X Values) vs. L (Fit Values) from the curve fit

ThermalExpansion 8:04:32 PM 11/20/15

|    | g p dyn/cm2 | g dp d/cm2  | tan delta | temp C | delta L  | stress .../cm2 | X Values | Fit Values |
|----|-------------|-------------|-----------|--------|----------|----------------|----------|------------|
| 0  | -2.6189e+08 | 8.0607e+08  | -3.0779   | 30.183 | -0.17700 | 16.973         | 30.183   | -0.177     |
| 1  | 1.9357e+08  | -1.2217e+09 | -6.3113   | 30.240 | -0.17200 | 8.6209         | 30.977   | -0.172     |
| 2  | -1.5685e+09 | 4.8950e+08  | -0.31208  | 30.301 | -0.17200 | 11.041         | 31.772   | -0.168     |
| 3  | -7.1448e+08 | 2.5245e+08  | -0.35332  | 30.387 | -0.17200 | 15.123         | 32.566   | -0.164     |
| 4  | -1.3806e+08 | 6.3613e+08  | -4.6075   | 30.467 | -0.17200 | 13.374         | 33.361   | -0.161     |
| 5  | -3.4596e+08 | 3.4576e+07  | -0.099942 | 30.553 | -0.17200 | 3.1170         | 34.155   | -0.157     |
| 6  | -1.8423e+09 | 1.3350e+09  | -0.72466  | 30.660 | -0.17200 | 29.127         | 34.949   | -0.154     |
| 7  | -3.3932e+07 | 1.9456e+08  | -5.7338   | 30.783 | -0.17200 | 2.8029         | 35.744   | -0.151     |
| 8  | -7.2027e+08 | 6.7588e+07  | -0.093837 | 30.915 | -0.17200 | 9.5933         | 36.538   | -0.148     |
| 9  | -1.4108e+09 | -2.8059e+08 | 0.19889   | 31.072 | -0.17200 | 19.425         | 37.333   | -0.145     |
| 10 | 7.9196e+08  | 1.3190e+09  | 1.6655    | 31.222 | -0.17200 | 6.6409         | 38.127   | -0.141     |
| 11 | -7.2207e+08 | -3.4615e+08 | 0.47939   | 31.360 | -0.17200 | 16.099         | 38.922   | -0.138     |

19) take the derivative (as above) of the two fit columns

Prompt

Derivative:

7 X Column

8 Y Column

9 Output Column

Cancel OK

|      | stress .../cm2 | X Values | Fit Values |
|------|----------------|----------|------------|
|      | C6             | C7       | C8         |
| 7700 | 16.973         | 30.183   | -0.17700   |
| 7200 | 8.6209         | 30.977   | -0.17266   |
| 7200 | 11.041         | 31.772   | -0.16869   |
| 7200 | 15.123         | 32.566   | -0.16401   |
| 7200 | 13.374         | 33.361   | -0.16109   |

20) Plot  $dL/dT$  vs. "X-values" Although still noisy, a clear trend can be seen (note that the experiment was from high T to low and the high T data still has some "start-up" issues (blue circle). If this were a plot for publication, considerably more time would be spent in choosing the "right" curve fit so that the derivative is as smooth as possible.

