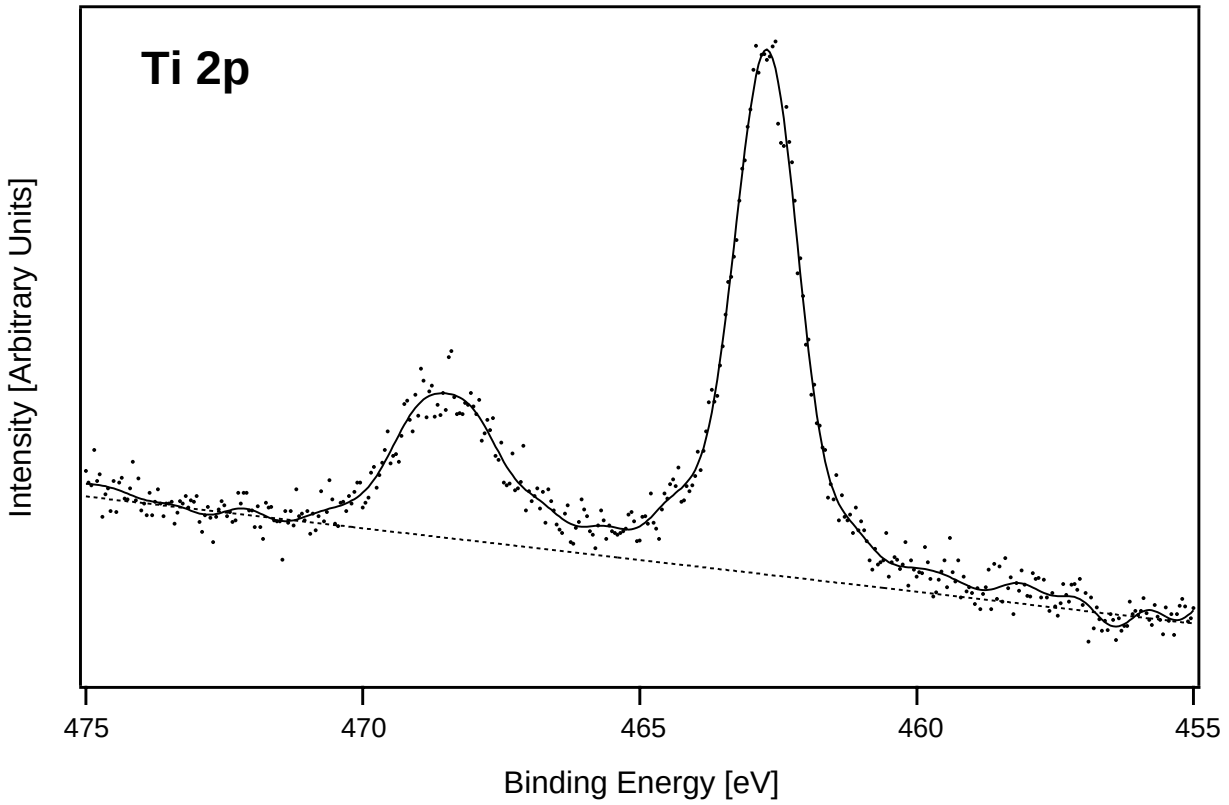
Homework 3

1. The graph below shows raw data, FFT smoothed data, and a linear background for Ti 2p peaks from XPS. The data files are posted on the Web as TigbRD (raw), TigbLB (linear background), and TigbSM (smoothed).



a. Determine the peak position and FWHM for the peak at lower binding energy from the smoothed data before and after background subtraction. Use whatever methods you deem appropriate. Please explain the methods briefly. Compare these results to those from part a and comment on whether the background subtraction has made a significant difference.

b. Determine the total area under the two peaks and the relative amount of area in each of the two peaks by whatever methods you deem appropriate.

2a. Smooth the data given in the table on the left using a simple 3 point smoothing algorithm. "Bounce" the values at the endpoints. The data are also provided on the Web as sampledata.

b. Repeat the smoothing operation using a simple 7 point smoothing algorithm. "Bounce" the values at the endpoints.

c. Compare the results of the smoothing operations by plotting the original data, the 3 point smoothed, and the 11 point smoothed on the same graph.

channel	value
0	-0.0294495
1	0.00512218
2	0.0130043
3	0.132714
4	0.167322
5	0.12639
6	0.253056
7	0.245613
8	0.411194
9	0.470754
10	0.536549
11	0.689198
12	0.826359

3. One way to represent a series of spectra from experiments under the same conditions is to make a composite spectrum, which is a sum of all the spectra divided by the number of spectra. The individual spectra

can then be compared with the composite spectrum to search for significant differences in peak parameters (peak heights, half-widths, and positions). This can be a considered a way to screen experimental results for possibly unsatisfactory results as well as a means of increasing the S/N ratio of the data (by co-adding spectra).

The following three spectra are XPS N 1s peaks from a nitrided Ti sample. They have been offset on the intensity axis for clarity - the raw data overlap. The peak at 401 eV is from hydrocarbons that contain N (RN peak), and the peak at 397.5 eV is from titanium oxynitride species (TiNxOx peak). The raw data are provided on the Web NpeakA, NpeakB, and NpeakC.

a. Make a composite spectrum from the three spectra.

b. Determine the ratio of peak heights for RN/TiNxOx from each of the three separate curves and from the composite curve. Tabulate the results. Comment on whether any of the peak height ratios from the individual curves appear to be significantly different from that for the composite spectrum.

c. Determine whether the S/N ratio has increased by a factor of 1.7 (square root of 3) in the composite spectrum as compared to the individual spectra.