FMRI RET 2017-Tunable Bandgaps of $WS2_{(1-x)}Se_{2x}$ Alloys

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Abstract

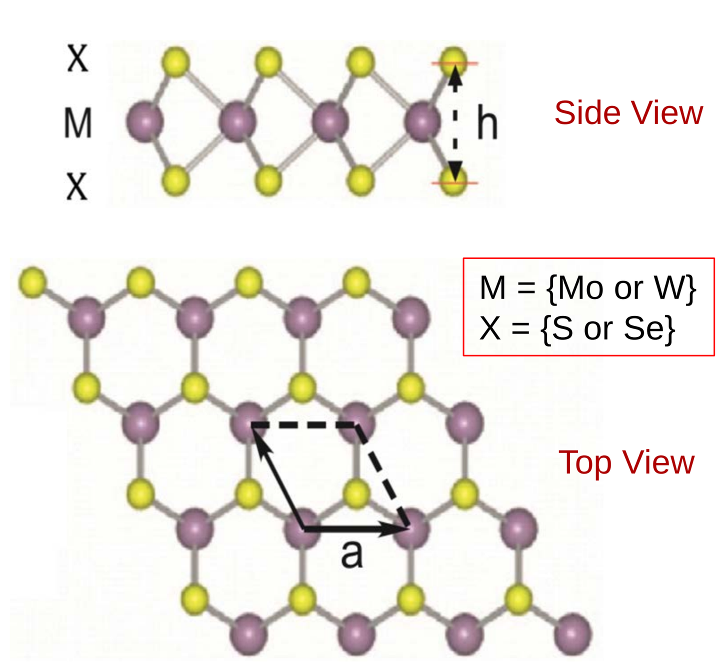
Monolayers of Transition metal dichalcogenides (TMDs) present a number of novel physical properties that make them attractive for applications in two-dimensional opto-electronic devices, including solar cells, diodes, and transistors. These materials have electronic bandgaps within the visible light spectrum. In this work, we have synthesized a variety of TMD samples based on ternary alloys where the chalcogen atoms (S and Se) are mixed in different concentrations to tune the bandgap of these films. This creates an opportunity to expand the range of the electromagnetic spectrum relevant to their future device applications.

Objectives

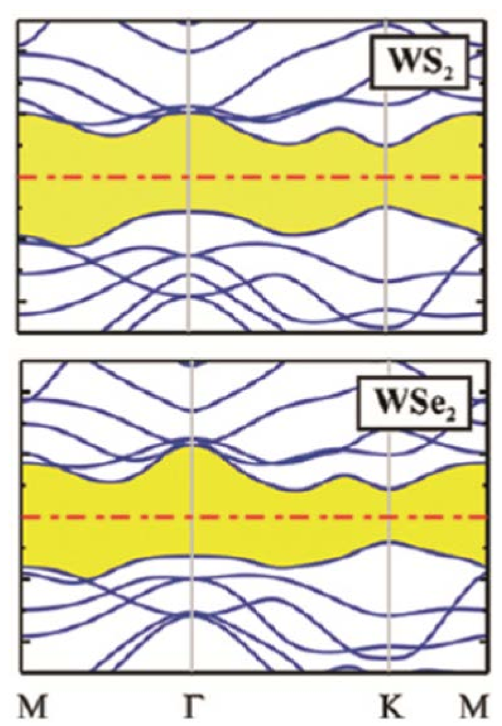
- To make monolayer large-area samples of varying TMD alloys with concentrations of WS2 and WSe2 shifting from pure WS2 to pure WSe2 using a modified CVD approach.
- Examine the samples with optical microscopy and Raman Spectroscopy to determine the coverage, morphology an composition of the sample.
- Determine the shape and spectral position of the exitonic peaks (optical bandgap) using Photoluminescence and optical Absorption spectroscopies.

Background

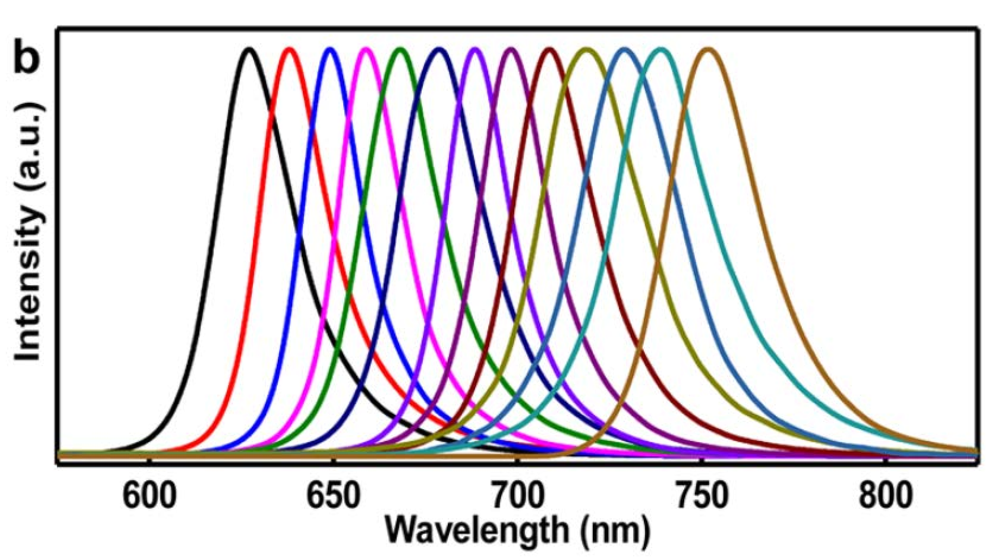
Crystal Structure

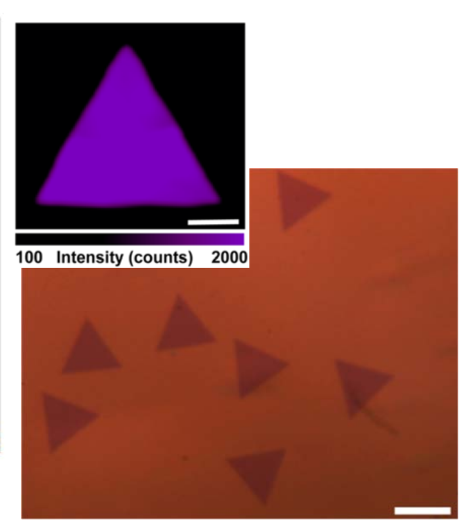


Electronic Structure



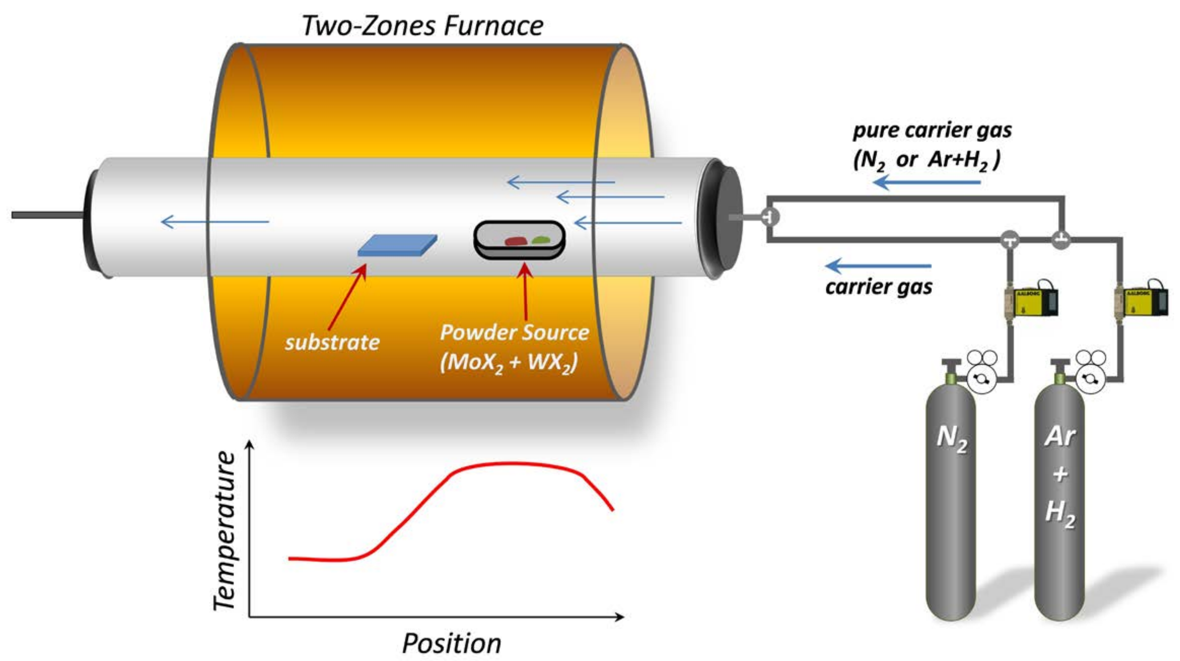
Ding et al., Physica B: Condensed Matter, Vol. **406**, p. 2254, 2011



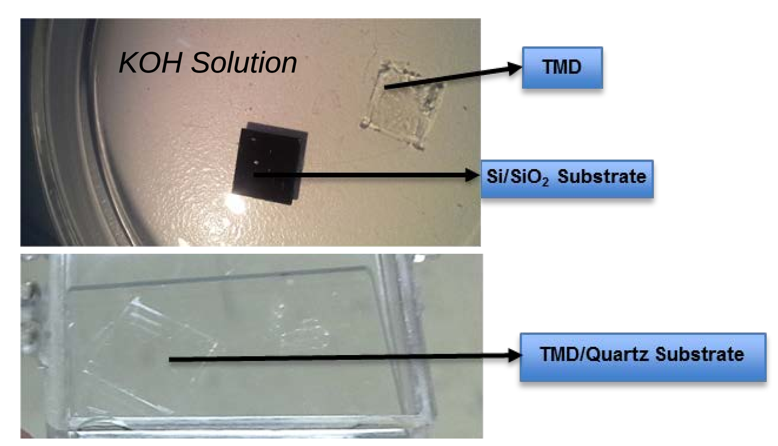


Duan et al., Nano Lett. 2016, 16, 264−269

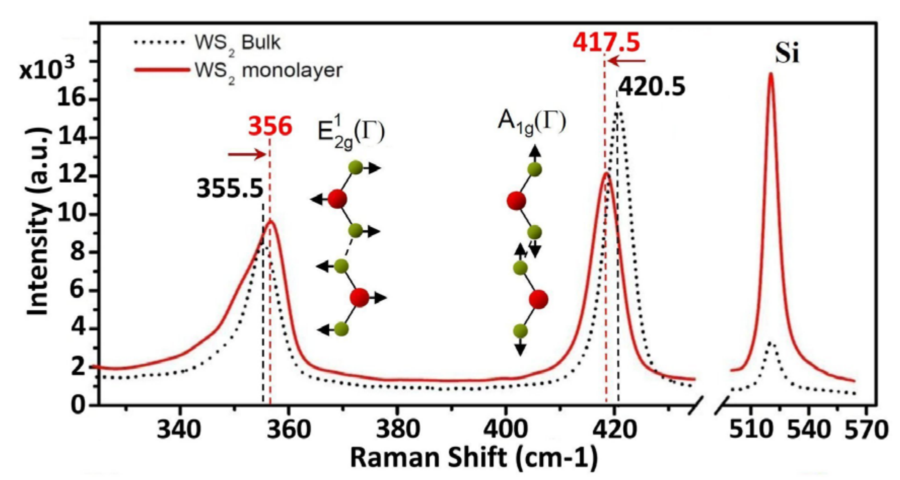
Approach



Physical Vapor Deposition (PVD) : The Si/SiO_2 substrates are placed in the furnace downstream from the boat containing the samples to be deposited. Some samples required both WS_2 and WSe_2 to be used, and in these cases the WS_2 was placed closer to the substrates.



TMD transfer to Quartz: The TMD is covered with PMMA by spin-coating to transfer the TMD to other substrates like quartz, sapphire, etc.

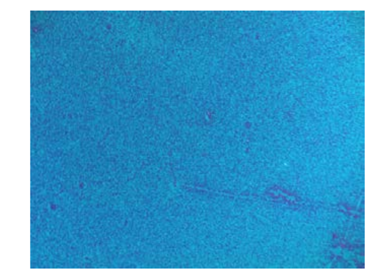


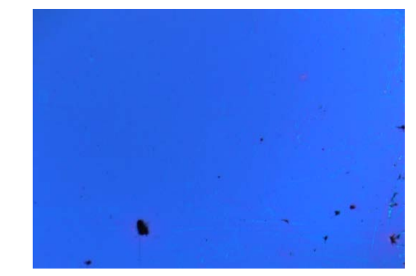
Raman Spectroscopy & Photoluminescence: The Raman spectroscopy shows us the different vibrational modes present in the sample. This allows us to identify the number of layers, gives an indication of the quality, as well as the substances present in the material. Photoluminescence gives us an indication of the bandgap for the material.

Conclusions

Eleven different samples of Tungsten dichalcogenide films were deposited on SiO2/Si substrates using a modified physical vapor deposition (PVD) technique. The samples consist of ternary alloys [WS2(1-x)Se2x] ranging from x=0 (pure WS2) to x=1 (pure WSe2). We performed a systematic study using Raman and photoluminescence (PL) Spectroscopies, as well as optical absorption. A shift in Raman peaks, consistent with the chemical composition of the samples, was observed. The shift of the excitonic peaks was studied both by PL and optical absorption, this behavior was then correlated with the growth conditions used to tune the chemical composition of the films. The results show a successful tuning of the electronic bandgap in atomically-thin TMD films.

Experimental Results



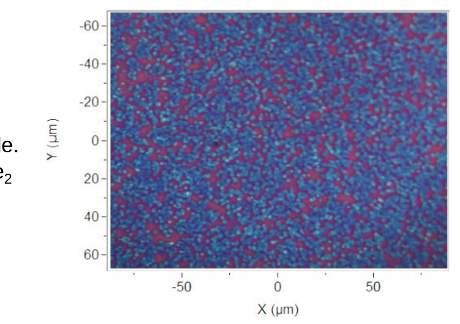


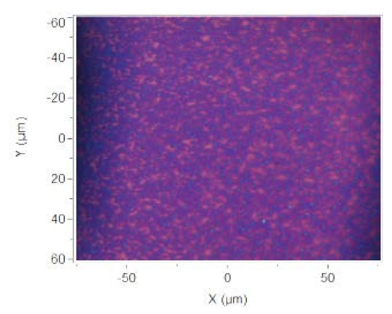
Images: Series 1 Growths

Bottom right: 100x image of 100% WS_2 sample.

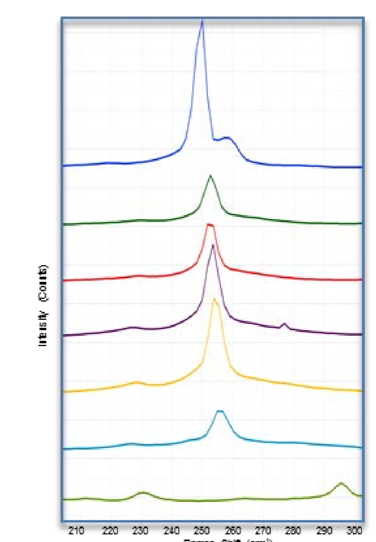
Top Left: 10x image of 100% WS_2 sample.

Top Right: 10x image of 50/50 WS_2/WSe_2 sample.

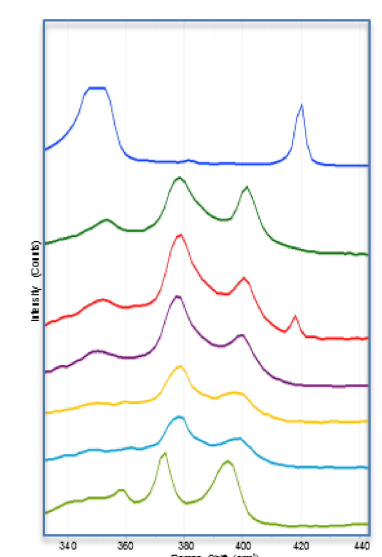




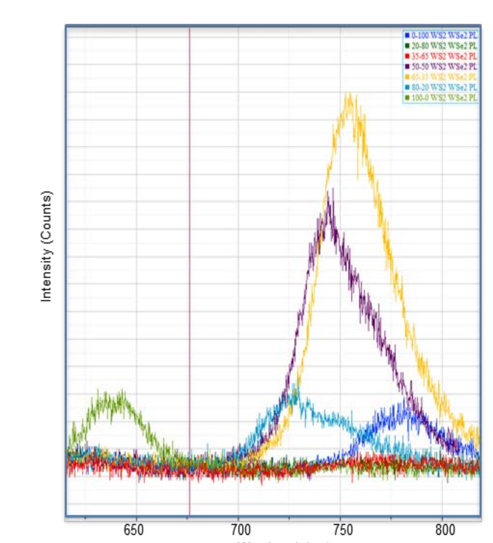
Series 1 Growths:
The image to the left was taken at 100x resolution of a growth done with 35mg of WS_2 and 65mg of WSe_2. The growths done in this series produced dusty clusters of multilayer alloys. Seven growths were done in the series ranging from pure WS_2 and the concentration of WS_2 decreasing as the concentration of WSe_2 increases.



Raman Shift:
The above graph to the left shows the WSe_2 peak at $250cm^{-1}$ and accompanying peak at $260cm^{-1}$. (Pure WSe_2 on top) The peak shifts towards the right (increasing) with the presence of WS_2. Until the peak disappears at pure WS_2.

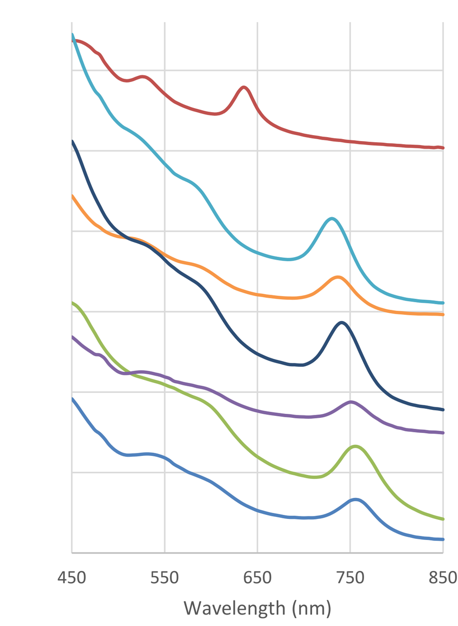


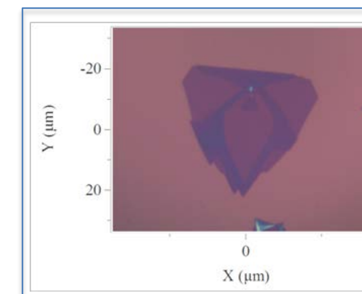
The above graph to the right shows Raman peaks for WS_2 at $350cm^{-1}$ and $420cm^{-1}$ (Pure WS_2 on top.) and the peaks for WSe_2 around $370cm^{-1}$ and $390cm^{-1}$ (Pure WSe_2 on bottom). The $350cm^{-1}$ peak shifts to the right as the concentration of WS_2 decreases, and new $WS_{2(1-x)}Se_{2x}$ peaks form around $378cm^{-1}$ and $400cm^{-1}$.



Photoluminescence (PL): The PL data for the seven growths is shown to the left. The dark blue is the pure WSe_2, and the light green to the left is the pure WS_2 sample. The samples shows a trend towards lower wavelengths as the concentration of WS_2 increased. All peaks required magnification due to poor coverage of the sample.

Absorption Data: The absorption data to the left is shown from pure WS_2 at the top, to pure WSe_2 at the bottom. The absorption data shows the same trend as the PL, as the concentration of WS_2 increases, the identifying wavelength decreases. All peaks required magnification due to poor coverage of the sample.



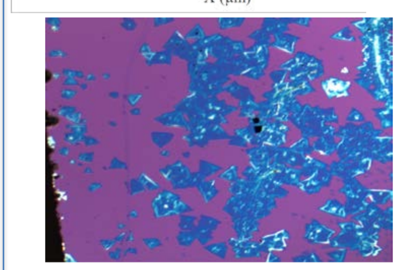


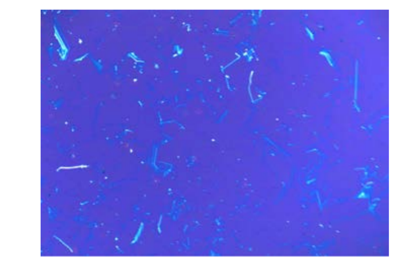
Images: Series 2 Growths

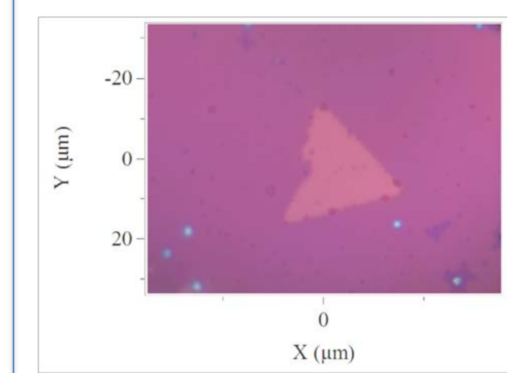
Left: 100x image of 50/50 WS_2/WSe_2 sample.

Bottom Left: 10x image of 50/50 WS_2/WSe_2 sample.

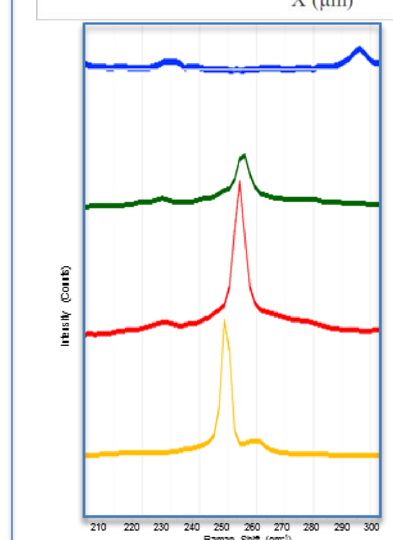
Bottom Right: 10x image of 75/25 WS_2/WSe_2 sample.



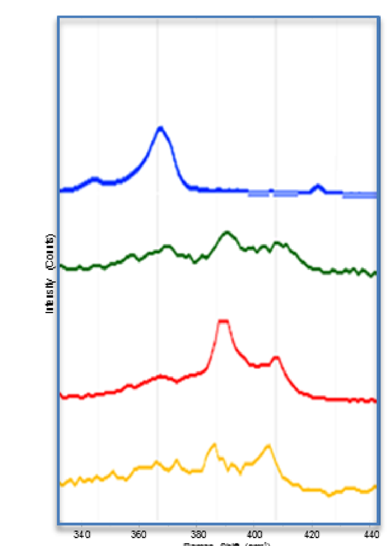




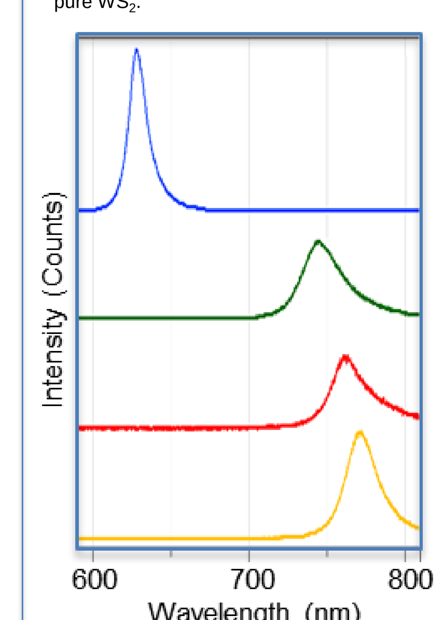
Series 2 Growths:
The image to the left was taken at 100x resolution of a growth done with 25mg of WS_2 and 75mg of WSe_2. The growths done in this series produced complete coverage of the substrates, with triangular islands of multilayer alloys, as shown to the left. Four growths were done in this series. All data below ranges from pure WS_2 at the top of the graph, to pure WSe_2 at the bottom.



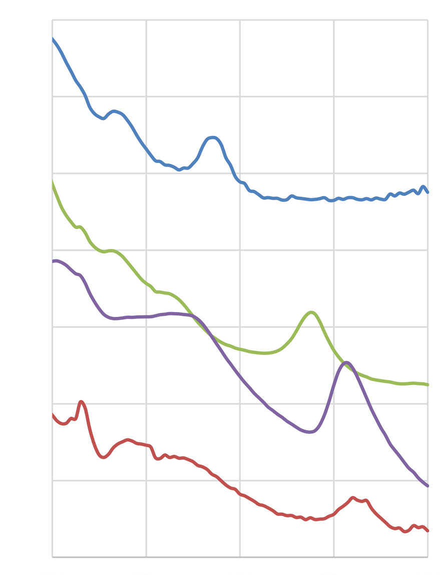
The above graph to the left shows the WSe_2 peak at $250cm^{-1}$ and accompanying peak at $260cm^{-1}$. (Pure WSe_2 on bottom) The peak shifts towards the right (increasing) with the presence of WS_2. Until the peak disappears at pure WS_2.



Raman Shift:
The above graph to the right shows Raman peaks for WS_2 at $370cm^{-1}$ and $420cm^{-1}$ (Pure WS_2 on top.) and the peaks for WSe_2 around $385cm^{-1}$ and $405cm^{-1}$ (Pure WSe_2 on bottom). New $WS_{2(1-x)}Se_{2x}$ peaks form around $390cm^{-1}$ and $410cm^{-1}$.



Photoluminescence (PL): The PL data for the four growths of the second series is shown to the left. The blue is the pure WS, and the yellow line on the bottom is the pure WSe_2 sample. The samples shows a trend towards lower wavelengths as the concentration of WS_2 increased. The PL of the second series showed much smoother peaks and required no magnification of the peaks because of the complete coverage of single layer.



Absorption Data: The absorption data to the left is shown from pure WS_2 at the top, to pure WSe_2 at the bottom. The absorption data shows the same trend as the PL, and the same trend as the first series; as the concentration of WS_2 increases, the identifying wavelength decreases. The absorption from the second series shows clearer peaks without magnification due to complete coverage since the system was cleaned between each growth.

For more information about the program visit: http://fmri-ret.eng.usf.edu/. The Research Experience for Teachers (RET) at the Functional Materials Research Institute at USF is funded by the National Science Foundation under award number 1301054. This research was also funded by NSF grant #DMR-1557434.